Data-Driven & Hybrid Models

KEYWORDS: Machine Learning/Hybrid Models/Physics-Informed Neural Networks/Scientific Machine Learning

This research presents advancements in applying machine learning, particularly Artificial Neural Networks (ANNs), to complex cyclic adsorption processes in chemical engineering. It highlights the limitations of traditional mechanistic models for real-time applications and proposes ANNs as a viable alternative. Specifically, it explores the use of Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTM) units for handling sequential data and long-term dependencies. The study also delves into physics-informed machine learning, employing Physics-Informed Neural Networks (PINNs) and Universal Differential Equations (UDEs) to solve complex numerical problems and integrate differential equations with data-driven models. This approach is applied to model industrial processes like column chromatography, offering innovative training methods for hybrid non-linear PDE problems. The findings provide new methodologies for addressing distributed-parameter problems in chemical engineering.

Introduction

Cyclic adsorption processes have very complex dynamic behaviour, which affects the development of strategies for the design, control, optimization, and inference of the process. Thus, it is difficult to use mechanistic models for real-time applications. Therefore, developing fast and accurate alternative models that capture complex dynamics is crucial.

Artificial Neural Networks (ANN) are empirical models that emerged as black-box alternatives to phenomenological models. It can approximate a variety of nonlinear functions at a low computational cost. In particular, Recurrent Neural Networks (RNNs) excel in processing sequential data, using their internal state for memory. However, they face challenges with long-term dependencies. Long Short-Term Memory (LSTM) units address this through gate mechanisms—input, forget, and output gates—that manage memory more effectively. This makes LSTMs superior for tasks like time series analysis, where understanding extended patterns is crucial. However, it has not yet found many applications in the field of chemical engineering processes, and we demonstrated the potential of this technology for the modelling of an industrial PSA process with complex dynamics.

The rising integration of machine learning in physical and natural sciences has steered research towards physics-informed artificial intelligence. Hybrid models in this domain are crafted to incorporate prior scientific knowledge, such as operational invariance and conservation laws, into machine learning, thereby introducing targeted biases that align with fundamental physical principles. Physics-Informed Neural Networks (PINNs) has been proposed as one of the ways to introduce prior knowledge into neural networks (a data-driven model). PINNs can address complex numerical problems, usually a limitation of the classic numerical methods, such as stochastic and high-order Partial Differential Equations. However, PINNs are based on the usage of the system conservation equations as constraints of a custom-designed loss function. Therefore, the design of the loss function plays a pivotal role in this technique. Following the peculiarities of the PDE system, supervised learning needs to be adequately designed. Thus, the PINNs methods should be carefully evaluated considering the application domain. Within this frame, we applied Physics-Informed Neural Networks (PINNs) to solve the numerical problem resulting from 1-dimensional mass balance in column chromatography. We study the peculiarities of these systems from the point of view of physics-informed neural networks, thus providing important initial guidelines to address adsorption-based models using PINNs.

Another important category of physics-informed machine learning lies in the concept of Universal Differential Equation (UDE). When differential equations, whether ordinary, algebraic, or partial, describe the underlying physics and are mixed with a data-driven model, the mathematical construct that emerges is termed a Universal Differential Equation (UDE). A universal approximator is an entity that can represent any conceivable function within a certain parameter size limit. In this context, Artificial Neural Networks (ANNs) stand out due to their ability to handle functions with high-dimensional input spaces and to become differentiable when equipped with suitable activation functions. However, applications have been limited to simple systems with few equations and poorly explored for more complicated problems, e.g., distributed-parameter representations such as fixed-bed reactors and chromatographic columns. In this sense, we developed a work that demonstrates a feasible and efficient way for training hybrid non-linear advection-diffusion-sorption PDE problems using gradient-based optimizers via continuous adjoint sensitivity analysis using quadrature adjoint with JIT-compiled tape-based vector jacobian product, orthogonal collocation on finite element PDE discretization scheme, and a fixed-leading coefficient adaptive-order adaptive-time BDF method ODE integrator.

Current Development

Regarding data-driven modeling of Pressure Swing Adsorption, twelve Artificial Neural Network (ANN) models were developed to adjust the H2/CO ratio in a syngas mixture using a PSA process illustrated in Figure 1.

Each model represented a different AI approach: classical, machine learning, and deep learning. The deep learning models, particularly LSTM-based DNNs, outperformed the others in predicting PSA dynamics, while classical and machine learning models, especially NOE, faced limitations in accuracy due to issues like gradient problems. The empirical models also achieved faster simulation times compared to phenomenological models, highlighting their potential for

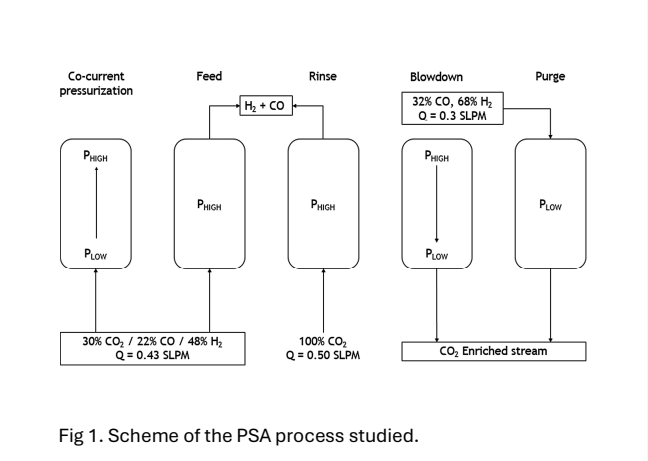

Fig 1. Scheme of the PSA process studied.

control, optimization, and real-time measurement strategies in complex dynamic environments. Figure 2 illustrates the different networks for CO2 purity, for the strong dynamics region (above) and the smooth dynamics region (below).

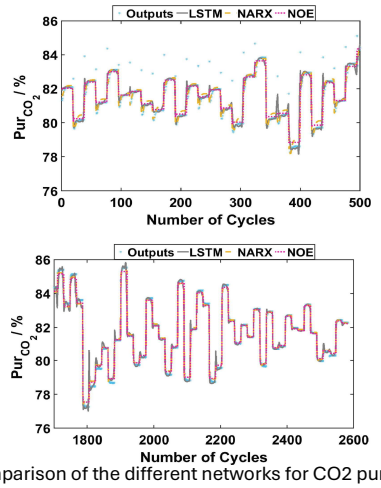

Fig 2. Comparison of the different networks for CO2 purity, for the strong dynamics region (above) and the smooth dynamics region (below).

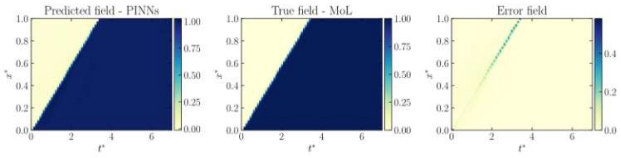

Fig 3. MoL and PINNs solution's comparison for adsorption experiment.

Regarding the PINNs development, the developed research is among the first to apply physics-informed neural networks (PINNs) to tackle numerical challenges in adsorption models, a novel area in chemical engineering. We demonstrated advantages of PINNs over traditional solvers by eliminating the need for complex spatial discretization, index reduction, and stiff system integrators. Demonstrated in fixed-bed protein separation, PINNs efficiently solved the adsorption process PDE, outperforming traditional methods in both accuracy and speed. Figure 3 depicts the comparison of PINNs with state-of-the-art solver. This work was developed under the cooperation of researchers from the Federal University of Rio de Janeiro and LSRE-LCM.

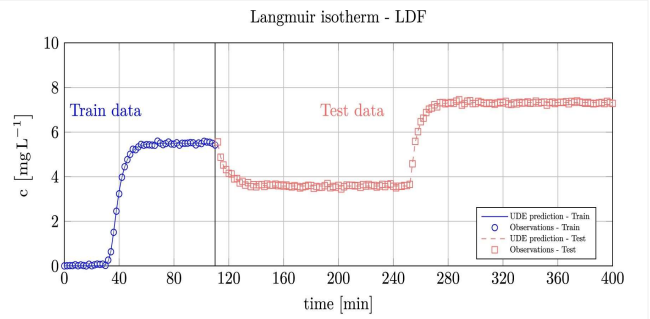

Fig 4. Results for Langmuir isotherm and LDF kinetics - 0.5 min-1 sampling rate.

In the UDE approach for advection-diffusion-sorption PDE problems, we demonstrated that the UDE approach fits breakthrough training data well, i.e., with errors compatible with simulated noise and with no apparent auto-correlation in time. Surprisingly, it also performs very well in the test set where desorption and adsorption from another steady state occur as can be seen from Figure 4. The results show that the ANN can learn adsorption uptake from single noisy breakthroughs at column outlet and extrapolate in adsorption and desorption well.

Future Perspectives

In terms of data-driven models, future works may consider new deep learning architectures used for natural language processing and large language models - transformers. For hybrid models, many questions are still open and future research may point to interpretability and scalability.

Related Sustainable Development Goals

Outputs

Master Dissertations

[1] Luis Miguel Cunha Oliveira, Modelling of a PSA unit by artificial neural networks, MIEQ, FEUP, 2019
[2] Guilherme da Costa Amaral, Model Topology Identification and Global Parameter Estimation for Purification of BSA and Myoglobin, MIEQ, FEUP, 2023

Selected Publications

[1] I. B. R. Nogueira *et al.*, Applied Soft Computing 67, 29-47 (2018)
[2] M. Karimi *et al.*, Ind. Eng. Chem. Res. 57, 259–267 (2018)
[3] L. M. C. Oliveira *et al.*, Chemical Engineering Science 224, 115801 (2020)
[4] M. J. Regufe *et al.*, Processes, 9, 1939, (2021)
[5] L. M. C. Oliveira *et al.*, AI, 2, 429-443, (2021)
[6] I. B. R. Nogueira *et al.*, The Canadian Journal of Chemical Engineering 100, 2279-2290 (2022)
[7] V. V. Santana et al., ChemEngineering 6, 21 (2022)
[8] E. Costa, *et al.*, Processes 10, 409 (2022)
[9] R. Santos et al., Separations 9, 43 (2022)
[10] C. M. Rebello, *et al.*, Processes, 10, 250 (2022)
[11] V. V. Santana *et al.*, Chemical Engineering Science 282, 119223 (2023)

Team

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