

Advancing Scientific Machine Learning in Physical Sciences: Applications in Process Systems Engineering



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MIT Portugal

2022 Annual Conference

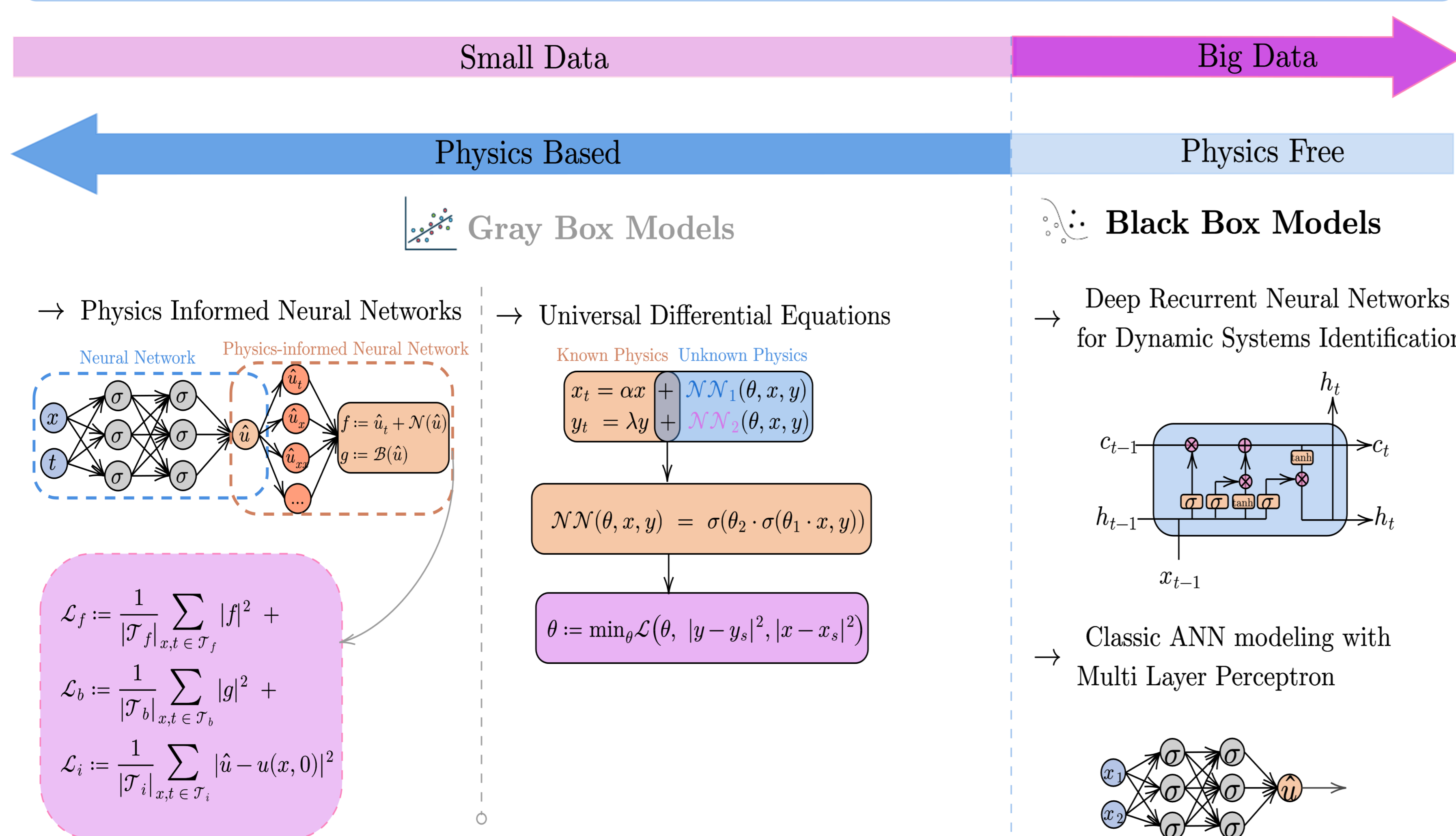
Introduction

Recent advances in machine learning and computer science started to drive important innovations in earth and life sciences. However, these developments have not yet found many applications in process systems engineering, where more “raw/pure” techniques are usually employed. “Pure” machine learning algorithms do not meet specific requirements for scientific applications– easy interpretability, generalization, and uncertainty quantification. The field of Scientific Machine Learning aims to develop the tooling for extracting interpretable and reproducible patterns from scientific data sets.

In this way, the current work aims to demonstrate state-of-the-art SciML tooling for process systems engineering with applications in:

- Column chromatography simulation with Physics-Informed Neural Networks (PINNs) [1];
- Column chromatography model discovery with Universal Differential Equations (UDE) [2];
- Chromatographic reactor model acceleration with Deep Recurrent Neural Networks;

Methodology



Results

Physics-Informed Neural Networks

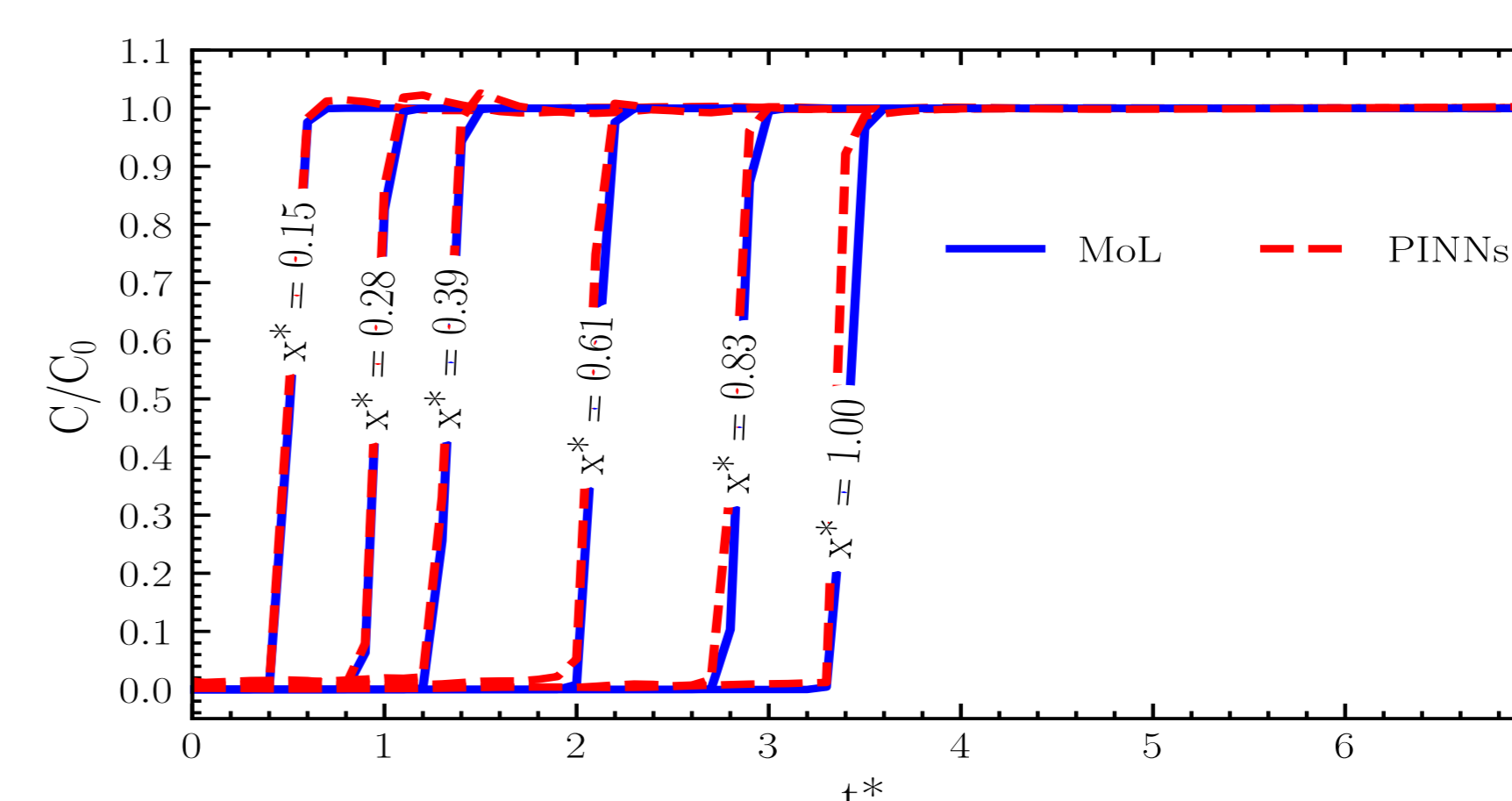


Figure 1. Method of lines and PINNs solution's comparison for adsorption experiment [1].

Universal Differential Equations

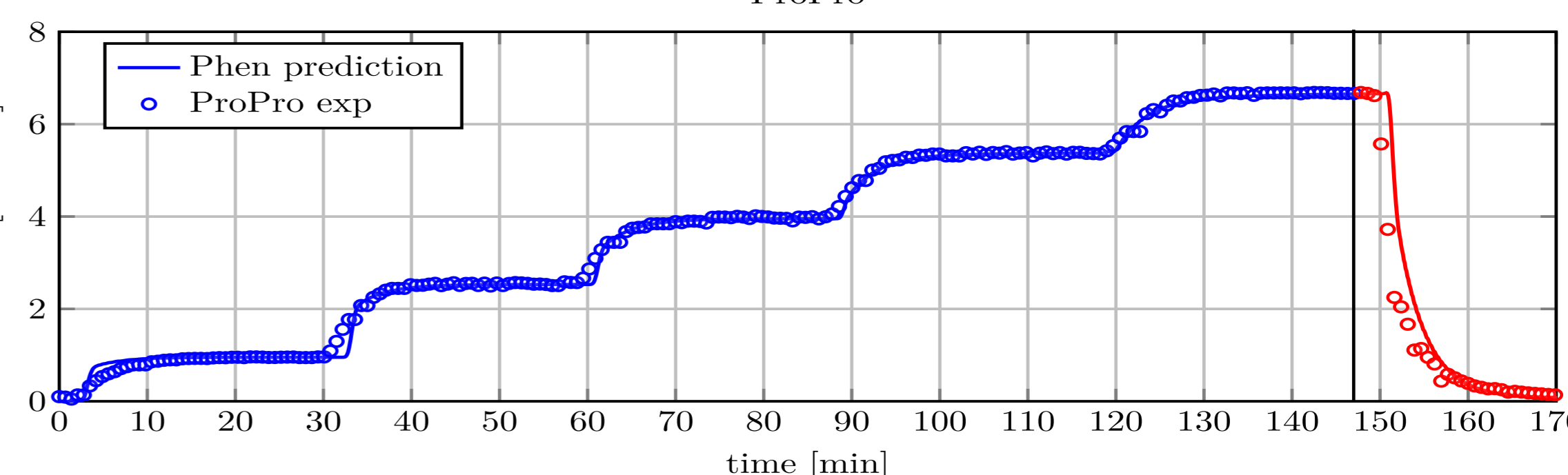
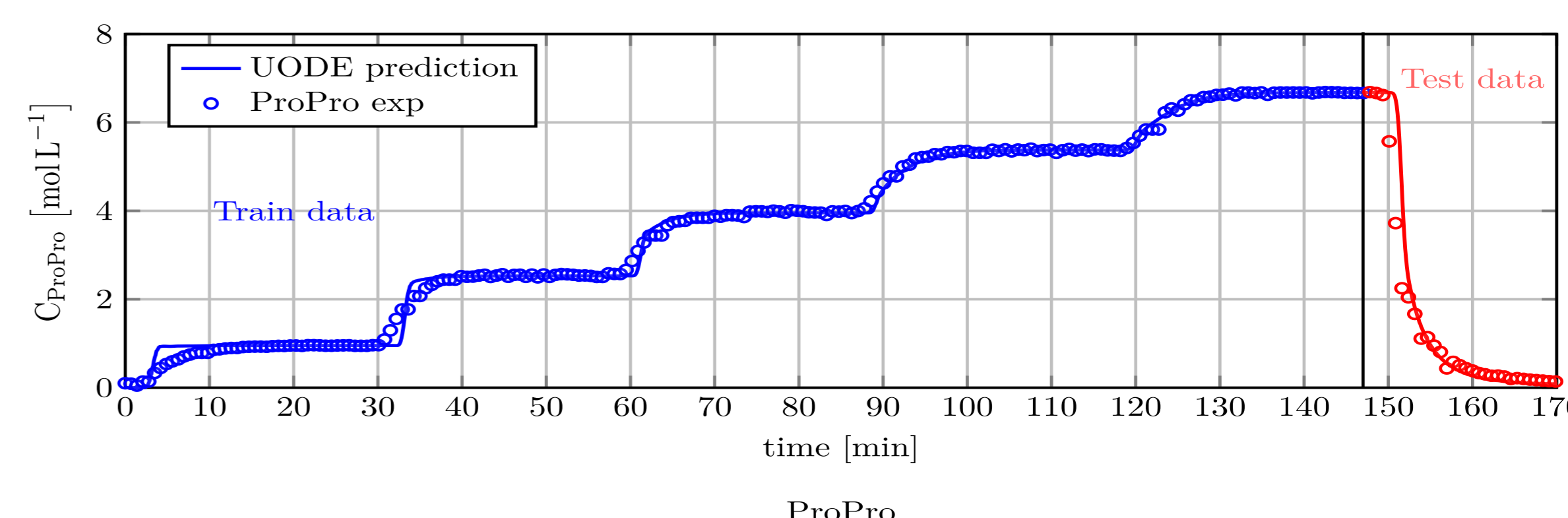


Figure 2. Train and test breakthrough curves for Propyl propionate – UDE vs Mechanistic comparison [2].

Deep Recurrent Neural Networks

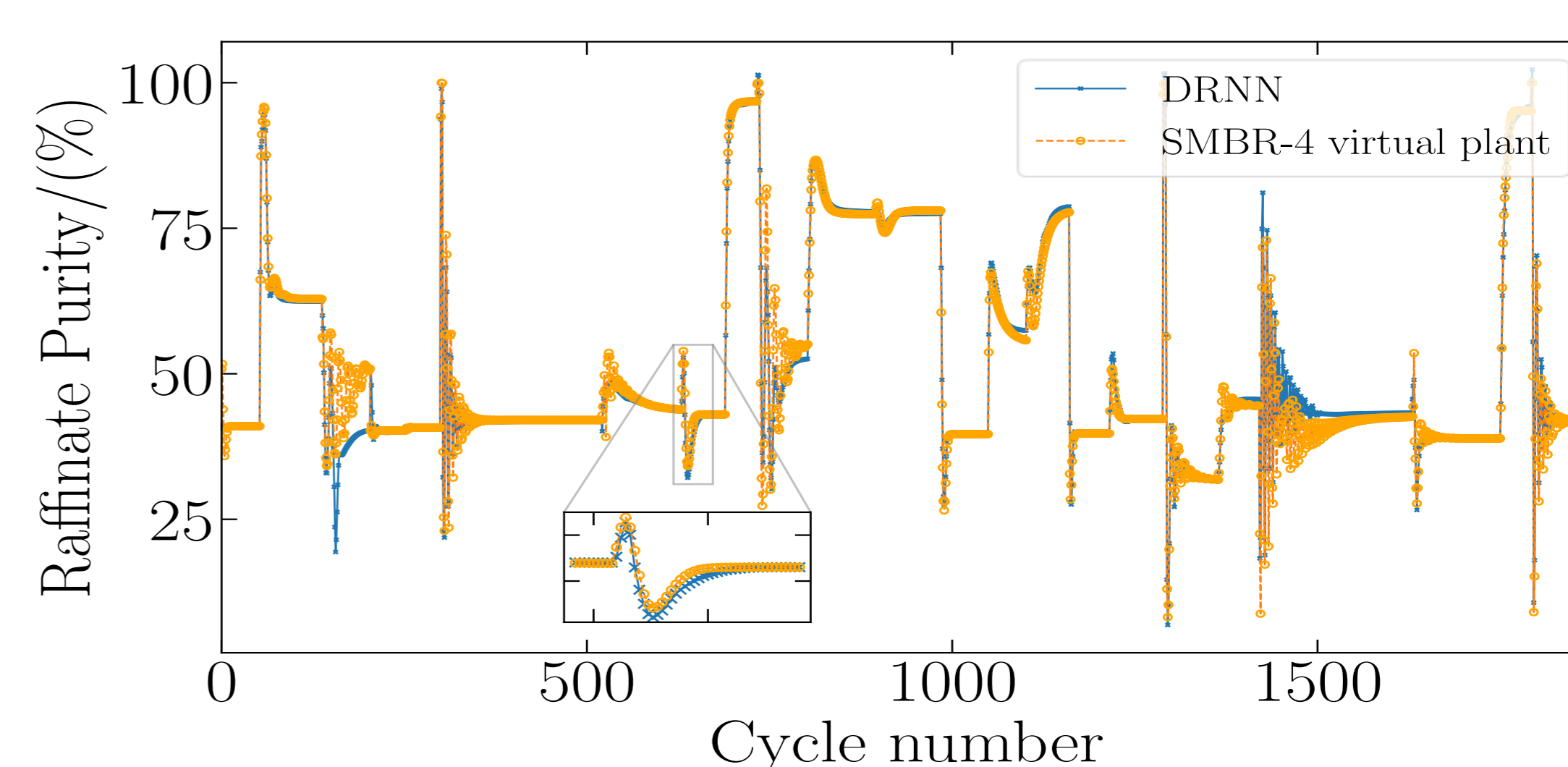


Figure 3. Comparison of DRNN predictions with virtual SMBR-4 plant in inference trial.

Conclusions

The three case studies successfully demonstrate novel applications of state-of-the-art sciML tooling applied to process systems engineering;

- The first case study was the novel demonstration of PINNs to simulate a column chromatography breakthrough experiment.
- The second case study demonstrates the superior predictive capacity of universal differential equations compared to entirely mechanistic modeling
- The third case study demonstrates how recurrent neural networks can provide a 4000x speed up in simulation time of chromatographic reactors with a prediction error of around 1%.

References

[1] Santana, V. V., Gama, M.S., Loureiro, J.M., Rodrigues, A.E., Ribeiro, A.M., Tavares, F.W., Barreto, A.G., Nogueira, I.B.R., 2022. A First Approach towards Adsorption-Oriented Physics-Informed Neural Networks: Monoclonal Antibody Adsorption Performance on an Ion-Exchange Column as a Case Study. ChemEngineering 2022, Vol. 6, Page 21 6, 21. <https://doi.org/10.3390/CHEMENGINEERING6020021>

[2] Nogueira, I.B.R., Santana, V. V., Ribeiro, A.M., Rodrigues, A.E., 2022. Using scientific machine learning to develop universal differential equation for multicomponent adsorption separation systems. Can. J. Chem. Eng. <https://doi.org/10.1002/CJCE.24495>