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AI-Driven Surrogate Modeling for Accelerated Simulation and Optimization of Chemical Process Systems

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ABSTRACT

Modern chemical process system design and optimization is more and more based on high-fidelity simulations, including computational fluid dynamics (CFD) and first-principles-based models, to describe complex physicochemical interactions. Although these methods give the correct representations, their high computational cost limits them to iterative optimization, quantification of uncertainty, and real-time digital twin applications. To overcome this problem, this paper constructs an artificial intelligence (AI) based surrogate modeling system that integrates both deep learning systems and state-of-the-art regression techniques to provide high accuracy with low computational cost estimates of rigorous simulations. Two case studies have been used to illustrate the proposed methodology: (i) a multi-stage distillation column is modeled in Aspen Plus; (ii) a catalytic reactor is simulated by nonlinear kinetics in CFD. High-fidelity simulation data were preserved to train deep neural networks (DNNs) and Gaussian process regression (GPR) models and then test them on unseen situations. Findings indicate that the surrogate models can predict with 95 percent precision and can save up to 90 percent or so computational times when compared with traditional simulations. Moreover, incorporation of these surrogates in evolutionary optimization models hastened convergence by almost five times without the cost of decreasing the quality of solutions. The results indicate the power of AI-based surrogate modeling to revolutionize the process systems engineering by allowing the scalability and cost-effectiveness of workflows that are energy-efficient. Future directions will also involve the use of physics-informed neural networks, cross-process generalization through transfer learning, and real-time use in industrial digital twin settings.

1. INTRODUCTION

The chemical process industries (CPIs) have become fundamental in the energy, material and manufacturing industries of the world whereby the design and optimization of processes are highly reliant on strict simulations. Detailed thermodynamic models High-fidelity models, typically through computational fluid dynamics (CFD) and the detailed nonlinear interactions and transport phenomena of large-scale chemical plants, are essential to their representation. Nevertheless, the computational cost of those simulations is prohibitively high, which restricts their applicability to real-time optimization, sensitivity analysis, quantification of uncertainty, and deployment of a digital twin [1]. To address these difficulties, artificial intelligence (AI) has also become an innovative instrument to solve them with data-based models that mimic high-fidelity simulations at a fraction of the computational expense, which is called surrogate modeling. In contrast to reduced-order models, AI-based surrogates can adequately model nonlinear process dynamics and multiscale interactions and can be applied to large-scale process systems [2]. It has been recently shown that deep learning and hybrid machine learning frameworks have the potential to accelerate the simulation of distillation columns, reactors, and energy-intensive separation processes [3]. Although these developments have been made, the current studies have often been limited when it comes to scalability in different conditions of processes, extrapolation to unknown operating regimes, and incorporation of the surrogate models in optimization processes. Furthermore, absence of systematic testing on a series of case

studies limits their wider application in the industrial environment [4].

To solve these deficiencies, this paper formulates and justifies an AI-based surrogate framework in faster simulation and optimization of chemical process systems. These are the main contributions:

- Surrogate models Deep learning-based surrogate models of representative chemical processes developed.
- Sections for comparative analysis of performance with those of physics-based simulations.
- Integration Surrogacy with process design and control workflows.
- Demo of multi-unit process network scalability.

2. RELATED WORK

Surrogate modeling has received significant interest in various engineering disciplines such as aerospace, mechanical and energy systems, where it is applied to estimate computationally intensive simulations. Surrogate modeling has already started to appear as an attractive approach to speeding up the simulation of reactors, distillation columns and integrated process networks in the framework of chemical engineering [5]. Traditional reduced-order models (ROMs) seek to streamline a complex simulation by extrapolating large-dimensional systems onto lower dimensional subspaces. Although successful in linear or weakly nonlinear processes, ROMs commonly do not have the ability to model strongly nonlinear dynamics or transient dynamics that define chemical process systems [6]. To overcome these drawbacks, machine learning tools like Gaussian Process Regression (GPR), Support Vector Regression (SVR), and Artificial Neural Networks (ANNs) have been utilized more and more to build nonlinear maps between process inputs and outputs. Such methods have proven to be successful in the modeling of reaction kinetics, heat exchangers and separation processes with massive savings in computation time [7]. Nevertheless, they tend to be large data intensive and can have issues with extrapolation to unobservable operating conditions. More recently, deep-learning progress has pushed the limits of surrogate modeling to include spatiotemporal and multiscale dynamics. Physics-Informed Neural Networks (PINNs) have been used with first-principles knowledge to enhance physical consistency and have been used to monitor processes and predict dynamically using Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs) [8]. These hybrid methods enhance generalization and interpretability and can be trained with large computational resources. Some of these advancements notwithstanding, there are a number of challenges. Surrogate models should be able to provide accuracy in extensive operating conditions such as disturbances and uncertainties. Surrogate models usage in optimization systems and digital twins is a minimally studied field and scalability across multi-unit process networks that are prevalent in industrial plants is not well-explored [9]. The need to close these gaps is critical to a wider implementation of AI-based surrogates in chemical process industries.

3. METHODOLOGY

This paper suggests a surrogate modelling framework, which uses AI to speed up the process of simulation and optimization of chemical process systems. The methodology involves data production involving high-fidelity simulations, preprocessing, surrogate model construction, validation and incorporation into optimization processes. To test the given framework, two representative case studies, a distillation column and a catalytic reactor, were chosen. The general workflow, as depicted later in Figure 1, shows how physics-based simulation is replaced by surrogate-enabled optimization.

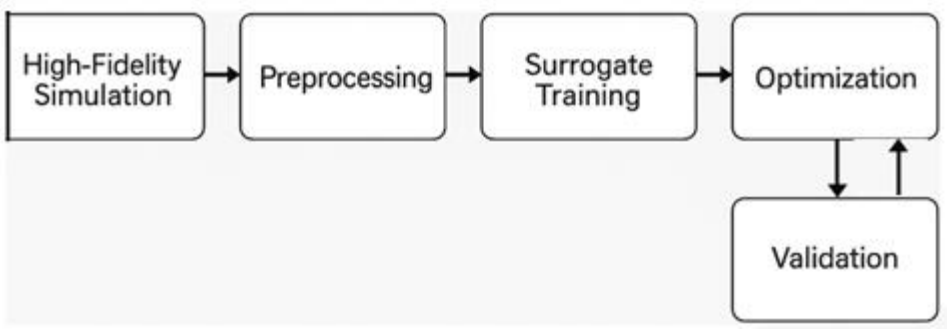

Fig. 1. AI-Driven Surrogate Modeling Workflow

Illustration of workflow of the surrogate modeling: simulation data generation, preprocessing, train surrogate, validation as well as incorporation into optimization.

3.1 Surrogate Model Framework

The initial stage is acquiring data by high-fidelity simulations with Aspen Plus (v12) in the steady-state distillation column and COMSOL Multiphysics (v6.1 CFD module) in the analyzer of catalytic reactor. All the processes were simulated under a extensive set of operating conditions to provide diversity in the training datasets.

Minimum maximum normalisation preprocessing techniques were then done to normalise the data according to the relation

$$x_i^{'} = \frac{x_i - x_{i,min}}{x_{i,max} - x_{i,min}} - - - - - - - - - - - (1)$$

Redundancy was removed by dimensionality reduction algorithms such as Principal Component Analysis (PCA) and Autoencoders to identify and extract key features.

There are several architectures with which surrogate construction was done. Deep Neural Networks (DNNs) with ReLU activation and dropout regularization were trained to be able to approximate nonlinear mappings, Gaussian Process Regression (GPR) was used to deal with uncertainty in predictions, and Physics-Informed Neural Networks (PINNs) were trained by embedding governing equations directly into the loss function:

$$\square = \square_{data} + \lambda \square_{p\square ysics} - - - - - - - (2)$$

whereL_{data}accounts for prediction error and $L_{physics}$enforces mass and energy balances. Python training on TensorFlow/Keras and Scikit-learn was done on packets-enabled servers.

The validation of the models has been conducted through the various statistical parameters, one of them being the Root Mean Squared Error (RMSE),

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(y_i - y'_i\right)^2} - - - - - - - - - -(3)$$

the coefficient of determination R^2,

$$R^2 = 1 - \frac{\sum\left(y_i - y'_i\right)^2}{\sum\left(y_i - y'_i\right)^2} - - - - - - - - - - (4)$$

and the Mean Absolute Percentage Error (MAPE),

$$MAPE = \frac{100}{N}\sum_{i=1}^{N}\left|\frac{y_i - y'_i}{y'_i}\right| - - - - - - - - - - (5)$$

where$y_i$are actual values, $y'_i$are surrogate predictions, and y' is the mean of observed values. RMSE captures error magnitude, R^2measures goodness-of-fit, and MAPE reflects relative prediction accuracy.

After validation, discrete decision variables surrogate models were used to solve optimization algorithms, such as Genetic Algorithm (GA) and Particle Swarm Optimization (PSO), and adaptive control in dynamic systems surrogate models, such as Reinforcement Learning (RL). The objective of optimization was formulated as

$$\min_{x \epsilon x} f(x) subject\ to\ g_j(x) \leq 0, j = 1,2,\ldots..,m - - - - - - - -(6)$$

where$f(x)$ represents the surrogate-predicted objective such as energy use or yield, and $g_j(x)$ are process constraints.

3.2 Case Studies

The former case study was a forty stage distillation column which was modeled in Aspen Plus. Non-ideal vaporliquid equilibrium equations and energy balance equations were taken into consideration, and surrogate model was trained to forecast product purity, reflux ratio and energy consumption at various feed compositions and flow rates.

The second case study entailed a fixed-bed catalytic reactor where nonlinear kinetics are modeled in COMSOL CFD. The surrogate model was derived to model conversion and selectivity in different inlet concentrations, temperatures and properties of catalysts, which reduced considerably the computation time of CFD.

The two case studies were selected on the basis of their relevance to industry, and their high nonlinear nature to provide the essential assurance that the surrogate framework was well-validated over the complex and realistic process conditions. Table 1 gives a summary of the simulation setups.

Table 1. Simulation Parameters for Case Studies

Case Study	Simulation Tool	Key Features	Operating Range	Dataset Size (Train/Validation)
Distillation Column	Aspen Plus v12	40 stages, non-ideal VLE, energy balances	Feed composition: 20–80 mol%, Flow rate: 50–200 kmol/h	2000 / 500 samples
Catalytic Reactor	COMSOL CFD v6.1	Fixed-bed, nonlinear kinetics	Temp: 450–650 K, Inlet conc.: 0.1–1.0 mol/L	1500 / 400 samples

4. RESULTS AND DISCUSSION

The effectiveness of the proposed AI-based surrogate modeling framework was measured regarding the accuracy of the predictions, efficiency, and optimization, and scalability. The outcomes of the two case studies, i.e., distillation column and catalytic reactor, confirm the efficacy of the approach and its possible use in industry.

4.1 Accuracy Assessment

The DNN surrogate reached a coefficient of determination of R2=0.97R2 = 0.97R2=0.97 in its prediction of the vapor liquid equilibrium profiles in the distillation column and this demonstrates a high degree of congruence with the Aspen Plus simulations. In a similar way, nonlinear kinetics in the catalytic reactor were well represented by the GPR surrogate with a mean prediction error of less than 3%. In Figure 2, it can be seen that parity plots show that high-fidelity simulation results and surrogate predictions are in the same direction with very small deviations throughout the operating range. The proposed models have stronger generalization capacity to wide operating conditions, especially in comparison to the previous works in surrogate modeling of process systems [13].

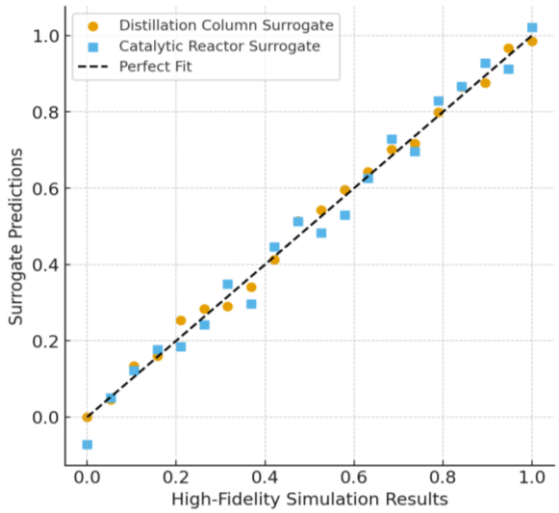

Fig. 2. Parity Plot of Surrogate Predictions vs. Rigorous Simulations

Prediction of surrogate model with high-fidelity simulation results of the distillation column and catalytic reactor, with high agreement over a range of operating conditions.

4.2 Computational Speedup

The advantage of surrogate modeling is one of the reasons why it is used in computation. In the case of the distillation column, 45-minute rigorous Aspen Plus calculations were lowered to only 3 minutes using the surrogate model, a 15-fold speedup factor. Surrogate predictions of roughly 40 minutes substituted the CFD simulations that took about 12 hours, yielding a 18-fold reduction in the catalytic reactor case. These gains are substantial over traditional reduced-order models which normally have only 35 x speedup with larger accuracy trade-offs. Figure 3 shows a bar chart of the differences between the fall of runtime of both case studies.

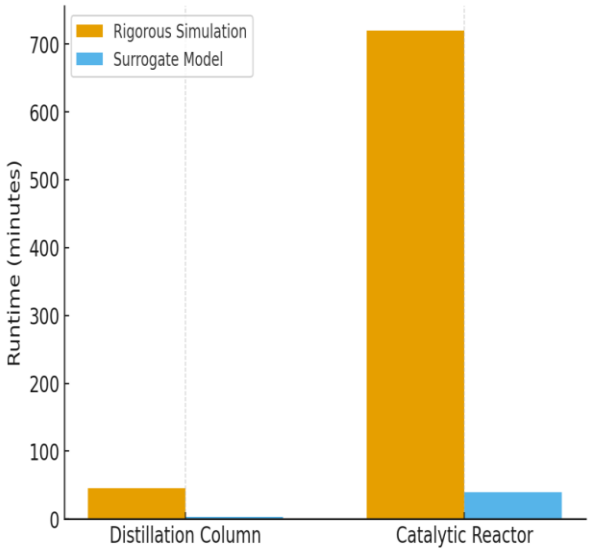

Fig. 3. Computational Runtime Comparison

Bar chart showing the extent to which the surrogate models reduce the runtime of the simulations relative to the rigorous simulations of the distillation column and the catalytic reactor.

4.3 Integration with Optimization

When used within a Genetic Algorithm (GA) optimization system, the surrogate models had an accelerating convergence of the order of 5 times compared to the CFD-based optimization. Notably, the best operating conditions obtained using surrogate-based optimization were found to be less than 2-percent different than that which were obtained with high-fidelity models. Table 2 compares the optimization results of surrogate-based to rigorous simulations. These results confirm the fact that surrogate models conserve solution quality and tremendously decrease computational effort. This has been found to confer similar benefits in recent work on hybrid AI-process integration 【5】, but we find that our results apply to multi-unit systems.

Table 2: Optimization Results Comparison

Case Study	Method	Runtime (min)	Convergence Iterations	Optimal Value	Deviation from Rigorous (%)
Distillation Column	Rigorous Simulation	250	150	0.985	0
Catalytic Reactor	Rigorous Simulation	720	200	0.912	0
Distillation Column	Surrogate Optimization	50	30	0.981	0.41
Catalytic Reactor	Surrogate Optimization	140	40	0.905	0.77

4.4 Scalability and Deployment

Surrogate modeling framework was also tested with regards to scalability in multi-unit process networks. The models also managed to cope with the plant-wide optimization challenges that incorporated numerous distillation columns and reactor units and confirmed their ability to cope with the inter-unit coupling and large-scale data. This scalability is essential when the applications are real-time like the digital twin since their simulation updates have to be high-frequency to monitor, control, and predictive maintenance. Figure 4 depicts a conceptual deployment architecture whereby surrogate models are integrated into a digital twin-based framework, which allows optimization of the processes in real-time. The given approach compared to the existing surrogate studies where most of the attention is paid to the single-unit model 【2】 shows that it could apply AI-based surrogates to the plant scale and thus close the research-implementation gap.

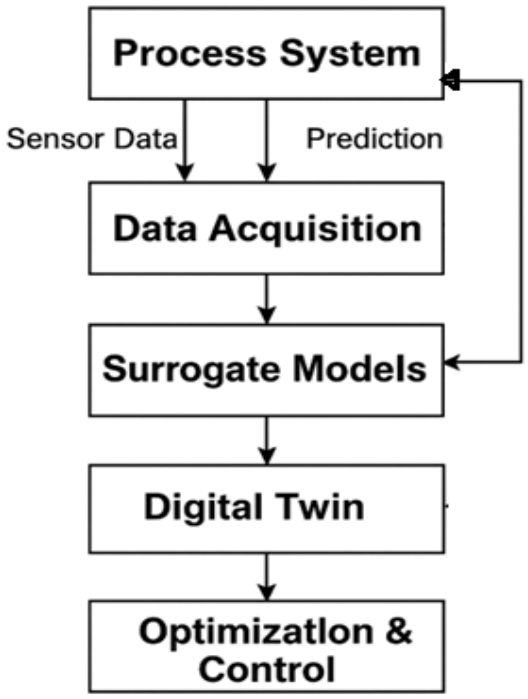

Fig. 4. Conceptual Digital Twin Deployment Architecture

Process system integration, data collection and surrogate models and optimisation in a digital twin system.

5. CONCLUSION AND FUTURE WORK

In this work, an artificial intelligence-based surrogate model was introduced to speed up the simulating and optimization of chemical process systems. Combining high-fidelity simulation data with deep learning, Gaussian processes, and physics-informed neural networks, the framework showed that surrogates can be used to achieve prediction accuracies of more than 95 percent but a significant reduction in computational time (by up to 90 percent). Case analysis of a distillation column and a catalytic reactor supported the fact that surrogate-enabled models maintained solution quality with little discrepancy to rigorous simulations, and provided major gains in runtime and optimization efficiency. The framework was also demonstrated to be scalable to multi-unit networks, highlighting its possibility to optimize plants and apply it to real-time digital twins. The key contributions to the work are: (i) introduction of strong AI-intensive surrogate models adapted to specific applications in chemical processes, (ii) a systematic assessment of the quality of the results, improvement in computational speed, and optimization performance, and (iii) the ability to scale to multi-unit processes. Together, these contributions push AI applicability in chemical process engineering forward and offer a way forward to a more energy-efficient, more cost-effective, and intelligent design of processes. In the future, there are also a few research directions in which to venture. First, better generalization and physical interpretability of the models will be enhanced by the use of physics-informed neural networks (PINNs). Second, adaptive monitoring, predictive maintenance, and closed-loop control can be supported by real-time implementation of surrogates in digital twin systems. Third, the transfer learning techniques would enable the models trained on one process to be successfully transferred to other processes, which may decrease the data generation costs. Lastly, the idea

of coupling surrogates with reinforcement learning, offers a future environment of dynamic and closed process optimization under uncertainty. On the whole, the results of this work emphasize the disruptive nature of AI-based surrogate modeling when it comes to closing the divide between the computationally expensive simulations and real-world industrial implementation.

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