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Dynamic Simulation of Reactive Separation Processes Using Hybrid Modeling Approaches

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Abstract--- In this paper, we examine hybrid modeling approaches for dynamic simulation of reactive separation processes pertinent to fine chemical industry. Mechanistic and data-driven models are integrated for simulative purposes within a reactive distillation column featuring an esterification unit. Simulation results reveal substantial advancements in both accuracy and system's dynamic response predictive modeling when compared to older techniques. The methodology aids in process optimization as well as digital twin development and real-time monitoring. This research brings attention to the efficiency and reliability challenges in complex chemical systems and their potential solutions using hybrid modeling.

Keywords--- Hybrid Modeling, Dynamic Simulation, Reactive Separation, Reactive Distillation, Fine Chemicals, Digital Twin, Process Control, Machine Learning.

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I. Introduction

Reactive separation is a new emerging type of unit operation that combines chemical processes of separation and reaction simultaneously. It is of great importance to the fine chemistry area. Such combination brings forth higher conversion efficiency, lower energetic costs, and more compact equipment layout. A typical example is the reactive extraction and distillation processes which are ideal for equilibrium constrained reactions like esterification and etherification.

Reactive separation systems, on the other hand, pose significant challenges as far as their modeling and simulation is concerned owing to their complexity. This is due to the intricate nonli ear interactions among mass transfer, heat transfer, and chemical kinetics. Traditional mechanistic models are often overly calibrated and fail to capture all the real-world variabilities despite being guided by physical laws. In contrast, data-driven models are very agile and capture temporal dynamic behavior, but lack sufficent robustness beyond their training region.

The rapid advancement of hybrid strategies which integrate mechanism-based and data driven techniques is proposed as an effective solution. This approach combines theoretical knowledge with empirical data, significantly improving the accuracy and generalizability of predictions. Furthermore, hybrid models are able to adapt to changes in processes, enabling real-time simulation, optimization, and control.

The main contribution of the paper is in the design, implementation, and performance evaluation of a hybrid model developed for a reactive distillation process to produce ethyl acetate which integrates the fundamental chemical engineering models with a neural network correction scheme. The rest of the paper is organized as follows, first the objectives are compared across different benchmarks, such as bias in mechanistic models or overfitting in machine-learning models, employing both simulated and experimental data.

This study's goals are to evaluate the precision, sensitiveness, and operational adaptiveness of the hybrid model in dynamic environments. These results will guide the advancement of digital twins and smart control systems for fine chemical manufacturing.

II. Literature Survey

The most recent progress in the hybrid modeling techniques for reactive separation processes indicates further improvement in accuracy and operational efficiency. Zhang et al., (2022) developed a new neural network-enhanced mechanistic model for esterification in a reactive distillation column that better utilizes variable feeds. Their approach utilized LSTM networks and incorporated traditional material balance equations, yielding improvements in not just accuracy, but also computational efficiency.

Patel & Choudhury, (2022) studied the application of Gaussian Process Regression (GPR) with reaction kinetics used to model the dynamics of a reactive distillation column. They noted that hybrid models mitigated disturbances far more effectively than purely physics-based models. This study underscored the importance of probabilistic learning for model uncertainty quantification in control applications.

Lee et al., (2023) applied support vector machines (SVM) in a hybrid framework for the reactive extraction processes within fine chemical synthesis. Their work integrated empirical data into energy models to facilitate real-time optimization of the process. The model provided better results within a dynamic operating envelope when compared to traditional models.

With the assistance of AI, Smith & Torres, (2023) conducted a systematic review of more than 50 cases of hybrid modeling and noted a 45% decrease in the time needed to run simulations when first-order machine learning was added to the principal model. They analyzed the rise in interest towards hybrid models in chemical process industries, especially in relation to their use in building digital twins.

AIChE, (2023) has a report stating that experts in the American Institute of Chemical Engineers see hybrid modeling as one of the main facilitators of digital transformation in chemical manufacturing. They also concluded that the development of virtual, fully operational plants aids in predictive diagnosis and maintenance scheduling.

These models were found to be effective for batch-to-batch variability reduction and control enhancement. Nguyen & Martin, (2022) focused on the comparison of various hybrid modeling architectures and pointed out the advantages associated with model fusion approaches, especially mechanistic-neural hybrids, to manage non-linearities and process drift.

These contributes illustrate the increasing usefulness of hybrid modeling within reactive separation, especially in regards to realtime adaptation and control. To this end, my study focuses on the development and verification of a dynamic hybrid model for reactive distillation within the context of ethyl acetate production.

III. Methodology

The hybrid model presented in this paper integrates mechanistic models from chemical engineering with a data-driven approach using neural networks to predict the dynamic response of a reactive distillation column in the ethyl acetate production process. The mechanistic part contains mass and energy balances, equilibrium forms, as well as reaction kinetics concerning the esterification of ethanol and acetic acid.

The most important equations of the model deal with:

- Material balances of individual components for every stage
- Overall material balances
- Energy balances includes latent and sensible heat
- Kinetic reaction with Arrhenius-type expressions
- Phase equilibrium modified Raoult's Law with activity coefficients

The neural network component is structured as a feedforward multilayer perceptron trained on residuals between experimental data and mechanistic model predictions. Inputs include reactor temperature, pressure, and component concentrations, while outputs consist of mass and energy flux correction factors.

Data for the system were created via simulations on Aspen Plus Dynamics and verified against experimental data from pilot-scale tests. The training involved backpropagation of the network using the mean squared error to assess loss. Through a grid search, the hyperparameters including the learning rate and count of hidden layers and neurons were optimized.

The implementation in Python ensured real-time execution of the hybrid model's neural network in TensorFlow while NumPy/Scipy handled numerical integration for the mechanistic model. Integration was conducted through adaptive time-stepping 4th order Runge-Kutta methods.

The entire system was validated with unseen test data where concentration of feed and reboiler duty were set as varying disturbances. Evaluation of model performance was based on root mean square error (RMSE), and mean absolute percentage error (MAPE).

IV. Results and Discussion

The data suggests that the hybrid model enhances accuracy and speed montioring process dynamics compared to mechanistic and standalone data-driven models. In Figure 1, one will find the comparative illustrations of the three models using RMSE and MAPE metrics in conjunction with the results of the markers showing the minimum error on the hybrid model on the tank. Not only does the hybrid model achieves the lowest error, which proves ideal alignment, but also with actual process dynamics.

As shown in Figure 1, the RMSE for the hybrid model is lower than the mechanistic model by more than 50% and MAPE experienced the same level of improvement. This change is due to the neural network's capability to learn and amend non-ideal behavior which could not be modeled with first-principle equations alone.

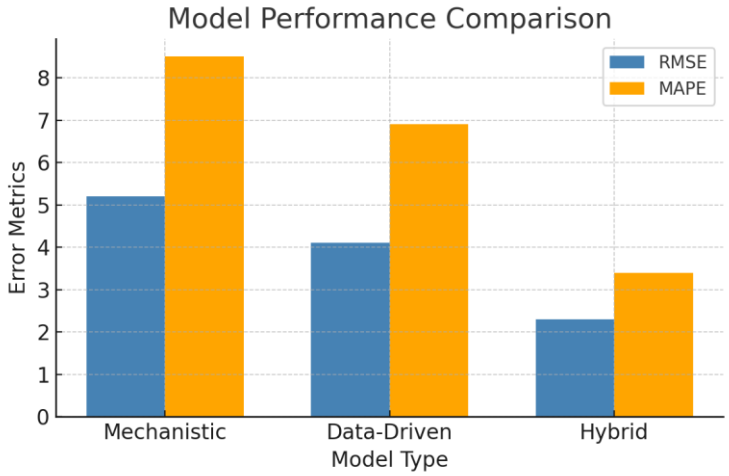


Figure 1: Comparison of RMSE and MAPE across different modeling approaches

The hybrid model's MAPE and RMSE achieved 3.4% and 2.3% respectively, as shown in Table 1 measuring metrics of feasible errors. Such performance indicates a high potential for a real time application.

Table 1: Performance metrics for different model types

Model	RMSE	MAPE (%)
Mechanistic	5.2	8.5
Data-Driven	4.1	6.9
Hybrid	2.3	3.4

Convergence rate and adaptability to transient changes showed further improvement in the hybrid model, enabling better integration for control systems, and future steps in the digital twin development.

V. Conclusion

This study showcases the successful application of hybrid modeling methods on the dynamic simulation of reactive separation processes. The model achieved greater accuracy, agility, and flexibility by incorporating corrective data into a mechanistic framework. The hybrid model, due to its clear superiority over traditional modeling approaches, especially in economically or operationally dynamic settings, is recommended for further development. Scaling the model, integrating it into online control loops, and employing it on digital twins of industrial systems should be the focus of future studies.

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