Empowering Engineering with Machine Learning: Hybrid Application to Reactor Modeling

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Résumé

Hydrocracking is a chemical process that breaks down heavy hydrocarbons into lighter, more valuable products, using feedstocks such as vacuum gas oil (VGO) or renewable sources like vegetable oil and animal fat. Although existing hydrocracking models, developed over years of research, can achieve high accuracy and robustness once calibrated and validated (1-3), significant challenges persist. These include the inherent complexity of the feedstocks (containing billions of molecules), high computational costs, and limitations in analytical techniques, particularly in differentiating between similar compounds like iso and normal alkanes. These challenges result in extensive experimentation, higher costs, and considerable discrepancies between physics-based model predictions and actual measurements.
To overcome these limitations, effective approximations are needed that integrate both empirical data and established process knowledge. A preliminary investigation into purely data-driven models revealed difficulties in capturing the fundamental behavior of the hydrocracking reaction, motivating the exploration of a hybrid modeling approach. Among various hybrid modeling frameworks (4), physics-informed machine learning was selected for in-depth examination, as it can leverage well-established first-order principles, represented by ordinary differential equations (ODEs), to guide data-driven models. This method can improve approximations of real-world reactions, even when the first-order principles do not perfectly match the underlying, complex processes (5).

This work introduces a novel hybrid modeling approach that employs physics-informed neural networks (PINNs) to address the challenges of hydrocracking reactor modeling. The performance is compared against a traditional kinetic model and a range of purely data-driven models, using data from 120 continuous pilot plant experiments as well as simulated scenarios based on the existing first-order behavior model developed at IFPEN (2).

Multiple criteria including accuracy, trend analysis, extrapolation capabilities, and model development time were used to evaluate the methods. In all scenarios, the proposed approach demonstrated a performance improvement over both the kinetic and purely data-driven models. The results highlight that constraining data-driven models, such as neural networks, with known first-order principles enhances robustness and accuracy. This hybrid methodology offers a new avenue for modeling uncertain reactor processes by effectively combining general a priori knowledge with data-driven insights.

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