

Mechanistic AI: Enhancing Accuracy and Interpretability of Soft Sensors in Advanced Process Control

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December 22, 2024

In modern refinery operations, precise and timely control of product quality is essential for optimizing performance and meeting stringent specifications. The Crude Distillation/Vacuum Distillation (CDU/VDU) traditionally relies on laboratory measurements for product quality assessment, with samples analyzed three or fewer times per day. This infrequent sampling is insufficient for closed-loop product quality control, which demands reliable readings at the control rate—typically once per minute. The absence of dependable on-line stream analyzers exacerbates the challenge, as existing analyzers often provide delayed responses unsuitable for multi-variable closed-loop control.

Soft sensors emerge as a vital solution to bridge this gap by establishing mathematical relationships between product quality and directly measured process variables. Common modeling techniques include regression analysis, artificial neural networks, and semi-empirical grey-box models. Serving as the "eyes" of an Advanced Process Control (APC) system, soft sensors enable real-time monitoring and control of product qualities without relying on delayed lab data or stream analyzers—these are utilized only for periodic calibration of the soft sensors.

Accurate soft sensors are crucial for the effective operation of APC systems, directly impacting the system's ability to maintain product quality within desired parameters. However, these methods have inherent deficiencies that can hinder their effectiveness. Traditional regression models often assume linear relationships between variables. Refinery processes are highly nonlinear and dynamic, involving complex interactions between multiple variables. Linear regression fails to capture these nonlinearities and interdependencies, leading to inaccurate predictions. Additionally, regression models are sensitive to collinearity among predictor variables, which is common in process data, potentially compromising the model's reliability. Although, such this shortcoming is addressable by partial least squares modeling technique, the underlying causality between variables will be obfuscated. Another widely used technique is artificial neural networks and while ANNs can model nonlinear relationships, they require extensive and representative datasets for training to generalize well. In the context of CDU/VDU units, the limited frequency of lab measurements means that available datasets are sparse and may not capture the full range of operating conditions. ANNs are also prone to overfitting, where the model learns the noise in the training data rather than the underlying process behavior, resulting in poor predictive performance on new data. Furthermore, ANNs are often considered "black boxes," lacking transparency and interpretability, which poses challenges for troubleshooting and gaining insights into process dynamics. Grey-box models are often offered as the compelling alternative to the aforementioned techniques. These models combine theoretical knowledge with empirical data, but they often rely on simplifications and assumptions that may not hold under all operating conditions. The accuracy of semi-empirical models can deteriorate when the process deviates from assumed conditions, such as changes in feedstock properties or equipment performance. They may also require significant effort to develop and maintain, including updating model parameters to reflect process changes, which can be resource-intensive.

Mechanistic AI offers a robust solution to these challenges by leveraging a general formulation of mass and energy conservation laws, rather than relying on detailed first-principle models. This design enables the prediction of measurable variables and the estimation of unmeasurable ones, all while maintaining reasonable model complexity. As a result, Mechanistic AI can close the loop from data collection to state and feed composition estimation—an

achievement typically unfeasible with detailed physics-driven models that are too complex for Kalman filter implementation. Additionally, the incorporation of fundamental physical principles helps regularize noise and reconcile inconsistencies in the data, allowing even low-quality datasets to be utilized effectively. Because of its underlying physics-based framework, Mechanistic AI models also generalize easily with minimal customization, ensuring they continue to produce valid results even with out-of-distribution data.

In contrast to traditional supervised machine learning models—which are usually non-transferable to other units, have unknown validity limits, are difficult to interpret, and cannot provide insights beyond the training data—Mechanistic AI offers unique features unattainable by other approaches. It combines data and physics in a novel way, producing reliable prediction and estimation results while providing deep insights into the system. Mechanistic AI is not only applicable in process control, requiring robust models, but also in predictive and prescriptive maintenance, necessitating a profound understanding of the system’s internal workings.

A significant advantage of Mechanistic AI over traditional machine learning models is its superior interpretability. Grounded in physical laws, Mechanistic AI models have structures and parameters that correspond to tangible physical phenomena, making them inherently understandable to engineers and operators. This transparency facilitates easier validation, troubleshooting, and acceptance by stakeholders who require insight into how predictions are made.