Special Issue

Machine Learning-Driven Kinetic Modeling in Chemical- and Energy-Related Processes

Message from the Guest Editors

Machine learning (ML) is transforming the landscape of kinetic modeling in chemical- and energy-related processes by introducing data-driven, adaptive methodologies capable of capturing intricate reaction dynamics.

This Special Issue aims to showcase cutting-edge advances in ML-based kinetic modeling, with a particular focus on the following topics:

- Bottom–up data-driven modeling strategies that extract mechanistic insights from experimental, industrial, or simulated datasets.
- Applications such as catalysis, combustion systems, electrochemistry, and reaction engineering, where traditional modeling techniques struggle with complexity or uncertainty.
- Real-time integration of ML models with digital twins, sensor networks, and process control systems to enable adaptive, scalable, and efficient process operation.

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