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Generalized Physics-Informed Deep Learning Framework for Chemical Process Modeling

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ABSTRACT

The incorporation of mechanistic, first-principles chemical unit operation models into process modeling frameworks remains computationally challenging. Mechanistic models governed by complex nonlinear systems of ordinary and partial differential equations are intractable for modern deterministic global solvers, particularly within large-scale nonlinear and mixed-integer nonlinear programming (MINLP) formulations. As a result, surrogate modeling approaches have gained increasing attention. However, conventional surrogate models typically rely on strong process-level assumptions, simplified physics, or extensive data generation, which limits their extrapolation capability, physical consistency, and reliability across feasible process operating regions. Physics-informed neural networks (PINNs) offer a promising alternative by embedding governing physics directly into the learning objective loss function, thereby reducing dependence on large, supervised training datasets while preserving governing physical laws. Existing PINNs implementations are typically formulated in a unit-specific or problem-specific manner. However, PINNs formulations lack modularity, transferability, and integration readiness for process modeling workflows. Therefore, a critical gap exists in the development of a highly generalizable and customizable PINNs framework applicable for diverse complex process unit operations. In this work, we develop a unified physics-informed deep learning framework for modeling complex process unit operations. The developed framework ensures governing physical consistency while maintaining flexibility across diverse nonlinear systems. Numerical stability is achieved through structured normalization and consistent dimensional scaling, enabling stable training across wide operating domains. A modular representation-agnostic architecture allows flexible specification of input-output dimensional spaces, systematic enforcement of boundary and operating constraints, and adjustable coupling between physics-based and data-driven loss objectives. Further, the developed framework promotes transferability and scalability across diverse modeling tasks by avoiding problem-specific architectural redesigning. Beyond predictive accuracy, the framework facilitates seamless integration of physics-informed surrogates within broader hybrid modeling workflows. Further, we validate the framework performance through multiple case studies, demonstrating robustness, scalability, and reduced reformulation effort relative to conventional PINNs implementations. This work advances physics-guided deep learning toward a reusable computational infrastructure for AI-enabled process chemical process modeling and simulation.