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Domain-Decomposition Pinns for Rapid Prediction of Stirred-Tank Mixing Flows across Geometric Scales

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ABSTRACT

Stirred-tank mixing is a central operation in batch chemical process design and scale-up. While high-fidelity Computational Fluid Dynamics (CFD) is effective for evaluating internal flow states, its computational cost prohibits its use in many-query tasks such as design-space exploration and parametric screening across varied equipment scales. Recent advances in Physics-Informed Neural Networks (PINNs) offer a promising path toward rapid surrogate modeling; however, conventional PINNs often fail to capture complex boundary conditions near impeller regions, frequently collapsing to trivial zero-velocity solutions due to dominant localized forcing terms. In this work, we present a data-informed, physics-constrained hybrid surrogate model for stirred-tank mixing within a bounded geometric-operating space. We employ a domain-decomposition approach: the complex impeller-region dynamics are represented through data-driven boundary conditions derived from a limited set of initial CFD simulations, while the bulk inertial flow field is reconstructed using physics-based constraints (Navier-Stokes and continuity equations). The model was evaluated across multiple stirred-tank specifications, including varying scale factors (1x, 1.5x, 2x) within the sampled design space. Results demonstrate that a single proposed model accurately reproduces three-dimensional velocity fields and mixing trends (RMSE = 0.0261), while reducing inference time by over 99% compared to repeated CFD simulations. Rather than functioning as an extrapolative general scale-up model, this framework is positioned as a local surrogate. By amortizing the initial offline CFD costs, it provides rapid, physics-consistent flow predictions for scale-related design analysis and operating-condition screening within an admissible interpolation domain.