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Learning Fluid–Particle Interactions: A Machine Learning Approach for Coarse-Grid CFD–DEM Simulation of Fluidized Beds

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ABSTRACT

Gas-solid bubbling fluidized beds are widely used in catalytic cracking, gasification, combustion, and other reaction-engineering applications because they provide strong gas-solid contact, vigorous particle mixing, and efficient heat and mass transfer. These desirable features arise from highly heterogeneous, multiscale hydrodynamics, which also make predictive simulation challenging. Fine-grid CFD-DEM can resolve local gas-particle interactions with high fidelity, but its computational cost becomes prohibitive for industrially relevant bed sizes, long physical times, and broad operating-condition coverage. Coarse-grid CFD-DEM therefore remains attractive for engineering-scale simulation, but its predictive capability depends critically on how unresolved gas-solid interaction forces are modelled. In bubbling beds, the vertical interaction-force contribution is strongly influenced by sub-grid heterogeneity, mesoscale structure, filtering level, and pressure-gradient effects that are not captured by a baseline drag law alone. The challenge is therefore not merely to improve drag fitting, but to develop a closure that is interpretable, dimensionless, solver-compatible, and transferable across operating conditions.

Overall, this study demonstrates that unresolved vertical interaction forces in bubbling fluidized beds can be learned as a base-drag-referenced and transferable ANN surrogate. The framework remains anchored to a conventional drag law, uses only solver-available dimensionless groups, and maps the learned target directly back to an effective drift flux coefficient Y_{drift} , making it suitable for ANN learning and deployment in practical scale-up coarse-grid CFD-DEM simulations. The combined evidence from particle-distribution analysis, transfer learning, F_z correction, and time-averaged solid fraction index prediction (Figure 5) shows that a data-driven machine learning can be used not only to improve prediction, but to identify an interpretable and reusable closure form that can be embedded into OpenFOAM-LIGGGHTS coupling solver. By formulating the correction using a pressure-inclusive two-branch network \mathcal{N}_{2B} instead of a pure black-box model of single-branch, the proposed architecture explicitly integrates physical knowledge, thereby improving prediction accuracy.

Future work will focus on leveraging transfer learning to generalize our pretrained neural network across different baseline drag laws, geometries, and fluidization regimes, where unresolved interaction forces continue to dominate coarse-grid model uncertainty. The resulting ANN-assisted simulations will be quantitatively compared with experimental measurements, whereby the corrected interaction forces are evaluated through macroscopic bed-scale observables such as pressure drop, bed expansion, solids holdup, and bubbling behaviour under matched conditions.

KEY WORDS

CFD–DEM, Machine Learning, Fluid–Particle Interaction

BIOGRAPHY

Ziyun Zhang is an undergraduate student in Chemical Engineering at the National University of Singapore (NUS). His research focuses on multiphase flow modelling using coupled CFD-DEM approaches, with an emphasis on integrating machine learning techniques to enhance simulation efficiency and predictive capabilities. Currently, his work explores particle-fluid interactions in complex systems, aiming to improve understanding and optimisation of industrial processes. He is interested in the intersection of data-driven methods and traditional engineering models, and aspires to apply computational tools to solve real-world scale-up challenges in chemical engineering.

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