Lattice Boltzmann Method CFD techniques applied to multiphase flow

Abstract

Multiphase flows play a key role in many industrial applications, particularly in the energy and chemical engineering sectors, where systems such as bubble columns and desalination units depend on complex interphase transport phenomena. Accurately simulating these systems remains challenging due to strong phase coupling, large density ratios, and the need for computational approaches that are both robust and scalable.

This doctoral work tackles these challenges through the development and application of advanced numerical frameworks based on the Lattice Boltzmann Method (LBM) and related computational strategies. Its main contribution is the formulation of a novel Eulerian–Eulerian LBM model that consistently recovers the volume-averaged Navier–Stokes equations for multiphase flows. Unlike traditional multiphase LBM approaches, the proposed framework enables an independent treatment of mass and momentum conservation for each phase, while incorporating physically consistent models for interphase momentum exchange. Particular attention is given to ensuring numerical stability in the presence of large density contrasts and to preserving the intrinsic locality and scalability of the LBM formulation.

The methodology is validated through systematic comparisons with reference finite-difference solutions and established benchmark cases. Furthermore, its extension to two-dimensional configurations is implemented within a GPU-accelerated framework based on JAX, demonstrating significant gains in computational efficiency.

Beyond multiphase flow modeling, the thesis explores the application of similar numerical principles within a classical CFD framework for membrane distillation. A pseudo-compressibility-based solver is employed to investigate heat and mass transfer in spacer-filled channels, with particular focus on temperature and concentration polarization phenomena and on the impact of spacer geometry on process performance.

Finally, this work explores emerging computational paradigms, with a particular focus on quantum computing. Preliminary investigations based on variational methods and quantum linear solvers are carried out on simplified transport problems, highlighting both the potential advantages and the current limitations of these approaches.

Overall, this thesis contributes to the development of scalable and physically consistent computational methods for complex transport phenomena, bridging mesoscopic modeling, conventional CFD, and emerging computing technologies.