International Conference on Numerical Combustion
Rome, Italy, October 14-17, 2025
www.icnc2025.com

Lattice-Boltzmann modeling of supercritical flows

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The present work investigates advanced modeling approaches for supercritical flows, particularly focusing on fluids such as CO_2 and N_2, which play an increasingly critical role in high-efficiency energy systems, including modern combustion technologies. The primary objective is to couple the Lattice Boltzmann Method (LBM) with a cubic equation of state to accurately capture the thermophysical properties of fluids in the supercritical regime.
While the LBM inherently supports the resolution of energy conservation equations, its direct application to thermally driven flows at supercritical conditions is computationally demanding [1]. To address this, recent developments have explored hybrid and double distribution function methods that aim to reduce computational costs while maintaining accuracy. However, many of these approaches assume ideal gas behavior and therefore fall short in modeling the non-ideal, nonlinear behavior characteristic of supercritical fluids—particularly near the pseudo-boiling region where compressibility effects become significant.
In this work, the use of a cubic equation of state, such as the Peng-Robinson model, is proposed to enhance the fidelity of simulations in capturing the thermodynamic behavior of real fluids under supercritical conditions. The proposed methodology lays the groundwork for simulating supercritical CO_2-based cycles used in waste heat recovery and oxy-combustion systems, where accurate representation of near-critical transport phenomena is essential for system optimization and control.
To further support applications in combustion-related systems, fluid-structure interaction techniques—such as the immersed boundary method—are integrated to study the behavior of solids interacting with supercritical flows, a situation relevant in heat exchanger design and combustion chamber cooling. The developed models are validated through academic benchmarks including entropy spot, Thermal Couette, Natural Convection and the Mayer's Jet test case.
This research opens pathways toward more efficient design and operation of combustion systems by improving the understanding of supercritical heat transfer and fluid dynamics.

References

[1] G. Farag, "Modélisation des écoulements compressibles via les méthodes Lattice-Boltzmann," in *Doctoral dissertation*, (Aix-Marseille University, 2022).