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(G*) Investigation of the Adsorption of Particles at Liquid-gas Interface: Numerical Modelling

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The dynamics of particles residing at a liquid-gas interface have shown to be of high importance both in fundamental studies and technological applications in recent years. Interfacial particles are amply found in artificial material manufacturing and biological systems. A better understanding of the unique physical properties of particles at the interface requires extensive attention to the surface interaction between the particle and the fluid. In this research, a computational method is employed to firstly successfully simulate the coexistence of liquid and gas, and secondly study the wetting properties of spherical particles at a liquid-gas interface. Different wetting boundary conditions will be tested to analyze the adsorption of the particle onto the interface. The simulations will be performed using a modified version of the lb/fluid package in LAMMPS, which is an implementation of Lattice Boltzmann method for simulating fluid mechanics. These results can provide us with enough insights to study interfacial particles with more complex conditions.

Keyword-1

Liquid-gas interface

Keyword-2

Interfacial particles

Keyword-3

Lattice Boltzmann

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