学 位 論 文 内 容 の 要 旨
DISSERTATION ABSTRACT

博士の専攻分野の名称　博士（工学）　氏名　龔 加明

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Numerical investigation of the free energy based lattice Boltzmann method for two-phase flow with large density ratio
(自由エネルギーに基づいた大密度比二相流体ラティス・ボルツマン法解析に関する数値研究)

Two-phase flows, especially the two-phase flow with large density ratio, occur in a number of important natural and industrial instances, such as petroleum exploitation, underground water recovery, fuel injecting in the internal combustion engine and ink injecting to the surface of paper, water removal from the fuel cell and so on. In order to accurately predict the their operation mechanisms and optimize design and operation of such systems, a better understanding of the two-phase flow from the numerical simulation is necessarily needed, owing to its flexibility compared with the experiment analysis.

The complex physics occurring in the interface involves a broad time and space scales for the two-phase flow systems. Essentially, the interfacial phenomena arise from the microscopic long-range interactions among the constituent molecules; and the thickness of interface between two phases is on the mesoscopic scale. The lattice Boltzmann method (LBM), which based on the mesoscopic kinetic theory, has become a popular tool for appropriately simulating the two-phase flows. Because of its kinetic nature, the microscopic intermolecular interactions can be incorporated into the LBM model in a straightforward way. Among the existing LBM models for two-phase flow, the free energy based LBM model is becoming more and more popular, due to its thermodynamic consistency. The early proposed free energy LBM model suffers the Galilean invariant problem for viscous term and is limited to small density ratio.

Among the recent proposed Galilean-invariance-free free energy models for large density ratio, the one proposed by Inamuro is simple and easy to implement, also it is able to simulate the two-phase flows with various density ratios below 1000:1. However, this model is poor in computational efficiency due to the iterative calculation of the approximate pressure Poisson equation; and also it contains some heuristic treatments whose effects on the simulation results have not been discussed in the literatures.

In this dissertation, the author starting from the basic LBM model for ideal gas introduced the fabrication idea of Inamuro's two-phase flow LBM model for large density. And then the author introduced the successive over-relaxation method (SOR) based formula and their corresponding staggered grids in solving the Poisson equation based fractional step method, which were adopted by Tabe et al. (2009) for easier implementation and faster calculation speed. In this process, the thermodynamic meaning of the pressure calculated in the Poisson equation is found to be the hydrodynamic pressure; and concept of the blending factor is introduced.

Focusing on the shape deformation and volume variation problem of a simulated static droplet in the quiescent gas phase, the author proved that the shape oscillation and volume expansion of the droplet in the steady stage comes from the numerical heuristic treatments of the 0- velocity inlet and free-out outlet boundary conditions which physically corresponding to the pressure constant boundary and such problems can be removed with adoption of the periodic boundary condition that corresponding to the volume constant boundary. Numerical analysis shows that the mass exchange at the 0-velocity inlet dominates the mass increasing in the computational domain, compared with the mass exchange at the free-out outlet.

The shape deformation and volume variation mechanism in the unsteady stage is analyzed with pe-

riodic boundary conditions to remove the disturbance from mass exchange with outside. The spurious velocity from the fractional step method is proved to be the main source of the shape deformation; and volume variation is proved to come from the diffusion process to form an appropriate interface and the diffusion process to equilibrium the pressure gradient and the interface tension across the interface. Besides, interaction between the diffusion effect and advection effect is found to be the minor source of shape deformation. With the use of the equilibrium order parameter in two phases, the droplet volume expansion can be greatly decreased and also the shape deformation caused by the diffusion can be reduced. Further, with the removal of the advection term from the equation, the shape variation tendency with the radii and the blending factor are totally removed; such numerical results prove that for the static equilibrium problem, the LBM model without the advection term may be a better choice.

The numerical error arising from the calculation of the Poisson equation based fractional step method with the two types of staggered grids is proved to belong to the category of the an-isotropic discretization error; which is one unique origin of the spurious velocity own in the present model; and the magnitude of the spurious velocity can be reduced to the half of the original value when the spurious velocity is free from the radius length effect, also the shape deformation can be minimized in this case. For the magnitude variations of the spurious velocity with the radius length, combining the initial diffusion process and the spurious velocity from the calculation of the hydrodynamic pressure, a reasonable explanation is given to illustrate how the magnitude of the spurious velocity changes and why the numerical phenomena that large shape deformation with small spurious velocity and small shape deformation with large spurious velocity occurs in the simulation. Moreover, the dependencies of droplet shape on the blending factor and droplet radii are summarized for the shape optimization.

The spurious velocity coming from the profile difference between the density ρ profile and the order parameter ϕ profile which is the main heuristic treatment in the present LBM model is also investigated. It is found that the density profile ρ in-continuous around the cut-off valve values of the two phases, the interface profile difference between the density ρ profile and the order parameter ϕ profile in the interface region and the interface thickness of the density ρ can separately induce spurious velocity. The density profile in-continuous around the cut-off valve values of the two phases induces the largest magnitude of spurious velocity when the derivative of the density ρ in the inter-molecular force terms directly make use of this profile and such type of spurious velocity can be reduced one order smaller and make the simulation stable by the adoption of a smooth profile based on the order parameter profile ϕ, compared with the original scheme. The spurious velocity arising from the interface profile difference can be decreased by the adoption of the liner magnification equation instead of the original sine type of magnification equation. And the incompatible discretization error and the an-isotropic discretization error are believed to be decreased by the increase of the interface thickness; thus further reduces the magnitude of the spurious velocity.