**Three-dimensional MRT pseudopotential multiphase LBM**

The simulation domain is Nx×Ny×Nz=200×200×250. Following Liu and Cheng, the saturation temperature of water is chosen to be *T*0=0.85*T*cr which corresponds to a liquid/vapor density ratio of 19.5. The parameters in the PR equation of state are set to *a*=2/49, *b*=2/21 and *R*=1. The surface is set to be smooth with a contact angle of 160º in order to eliminate the morphological effects on droplet jumping. Half-way bounce back boundary condition is applied on the solid surfaces.

All the variables are represented by lattice unit in the LBM simulations. To relate them to real physical properties, the constant Ohnesorge number *Oh* in lattice unit are equal to that in real unit, i.e., [*Oh*]lu= [*Oh*]real.(利用这个式子去关联模拟的液滴半径和实际的液滴半径) The Ohnesorge number  (, ,  and *R*0 are the water dynamic viscosity, density, surface tension and initial droplet radius, respectively), denotes relative effects of viscous and capillary-inertial effects that dominate the merging process. The properties of the droplet is taken as water at 20 °C, such as *ρ* =998.23 kg/m3, *σ* =72.75 mN/m, *μ* = 1.0087 mPa⋅s.（实际液滴参数）

模拟液滴参数：表面张力0.18299，密度6.698

Niu = (tau - 0.5)/3 *μ = Niu \* 密度*

For the radii of droplet considered in this work are much smaller than the capillary length, so the gravitational effect is neglected. 模拟中重力忽略了，因为模拟的液滴半径较小。

The three-dimensional nineteen-velocity (D3Q19) lattice Boltzmann model with MRT collision operator is considered. The evolution equation of LB model with the MRT collision operator is written as

 (1)

where  is the density distribution function, **x** is the spatial position, and  (*i*= 0,1, . . . 18) is the discrete velocity along the *i*th direction,  is the equilibrium distribution that can be written as

 (2)

where *w*0=1/3, *wi*=1/18 for *i*=1­-6 and *wi*=1/36 for *i*=7­-18. For the D3Q19 lattice model, **e***i* can be given as

 (3)

The collision matrix  in Eq. (2) is given by , in which **M** is orthogonal transformation matrix and **S** is a diagonal matrix given by (for the D3Q19 lattice)

 (4)

In the present work, we set , , , ,  and , where  is the relaxation time. （只改变松弛时间，其他的参数不要改）

The density distribution function  and its equilibrium distribution  can be projected onto moment space via  and , respectively. The equilibrium distribution functions  in the moment space are given by

(5)

where ,and are the momentum fluxes. Thus, the evolution equation of density distribution function can be rewritten as

 (6)

The collision step is implemented in the moment space and the distribution functions after collision is given by .

Then, the streaming process is implemented as

 (7)

where the force term  is incorporated through the exact difference method (EDM) as

, (8)

with  being the velocity change due to the force term **F** during time step . The density and velocity of the fluid can be obtained by

, . (9)

The whole fluid velocity is given by

. (10)

The force acting on the fluid **F** consists of the fluid–fluid force **F**int, the fluid–solid interaction force **F**ads and the body force **F**g.

For single-component multiphase flows, the interaction force **F**int mimicking molecular interactions is given by

 (11)

where  is the weight coefficient, *G* is the interaction strength.  is the interaction potential which is a function of the local density and is determined by the equation of state:



The wettability of the solid wall can be conveniently implemented by introducing interaction force between the solid and the fluid, given by



where  is the fluid–solid interaction strength for adjusting the contact angles.  is the indicator function,  when **x** is in solid and  when **x** is in fluid.

The body force **F**g is calculated by



where *g* is the acceleration of gravity and  is the density of the vapor phase. 模拟中重力忽略了，因为模拟的液滴半径较小。

In the simulations, the Peng–Robinson (P–R) equation of state is used, given by



where and  is the acentric factor which equals to 0.344 (the acentric factor of water). The critical properties can be obtained by



where  and  are critical temperature and critical pressure, respectively.