Multiphase Flow Modeling using Lattice Boltzmann Method

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Abstract—**To model the Multiphase flow along with phase transition process is a challenging task. In the present paper, capability of Lattice Boltzmann method (LBM) to simulate flow through complex geometries and multiphase flow has been discussed. LBM is an innovative computational fluid dynamics (CFD) approach based on kinetic models. It describes the physical system as an artificial micro-world of the particles in which the particles simply propagate, collide and interact. To check the validity of LBM, simulations have been performed for two dimensional Poisuelle flow as a test problem and compared with analytical result. Then simulations results for various geometries resembling the porous media, introduced in the flow have also been presented. For the simulation of multiphase flow involving phase transition Shan and Chen model has been used. Periodic boundary conditions have been applied in all directions. Then gravity has been introduced as the driving force. Phase transition occur spontaneously whenever the interaction strength between the particles exceeds its threshold limit. Results have been verified by Laplace law. Finally, it has been concluded that LBM is a simulation method of choice for simulating flow through porous media and multiphase flow.**

I. INTRODUCTION

Lattice Boltzmann method (LBM) developed in late 1980s is a powerful competitor of conventional CFD techniques especially in the era of multiphase flow ([1],[2],[3] and [[4]) (e.g. water and its vapors) and flows through complex geometries such as those present in porous media [5],[6].

Multiphase flow is of great industrial importance, especially for chemical engineers. Many operations such as catalytic reactions, floatation and gas absorptions involve two phases. Bubble dynamics significantly affects the rate of heat and mass transfer in many processes [7]. Simulation of fluids through complex geometries is crucial for the oil recovery wells since oil flows through haphazard paths [8].

LBM is based on Boltzmann equation and describes the physical system as an ensemble of fictitious particles. The hydrodynamics is demonstrated by the propagation of these particles in space and their collision with each other. These particles move at different velocities and their velocities change after their collision. Their microscopic behavior is reflected on the macroscopic scale by quantities such as density, velocity, viscosity, pressure etc.

LBM has several attractive features which distinguish it from other CFD techniques. Due to its kinetic nature, it provides a clear physical picture of the flow system. Its kinetic nature links it to the microdynamic flows, whereas, it can also recover the macroscopic Navier-Stokes equation in the incompressible limit, so it is regarded as a mesoscopic approach linking both the microscopic and macroscopic flows. The convection term in LBM is linear, unlike other CFD approaches, which reduces computational time and complexity. The pressure is computed through an equation of state rather than solving poisson equation, which is most time consuming task in traditional CFD methods [7].

To deal with complex boundaries is an easy job for LBM, whereas in other CFD methods, it is a big challenge. Due to linear convection term and local non linearity (if there is any for some specific case), LBM is a good host for parallel computing [9].

Kinetic nature of LBM makes it a powerful tool for modeling multiphase flow. To simulate multiphase flow, it introduces the interaction potential between the particles and phase segregation takes place spontaneously when this interaction exceeds its critical limit.

Since, there is no model without drawbacks. LBM also has some limitations. It is limited to low Reynolds number flows. In the simulation of multiphase flow, LBM is limited to low density ratio. Both limitations can be overcome by using multi-relaxation time which is difficult task.

II. LATTICE BOLTZMANN METHOD

Lattice Boltzmann method or LBM can be derived from Boltzmann equation after discretization. Boltzmann equation describes the particle transport from one node to the other by the continuous particle distribution function which is the number density of the particles moving with certain velocity at a certain time and space. The well-known Boltzmann equation is:

$$\frac{\delta f}{\delta t} + \mathbf{v}.\nabla_{\mathbf{x}} f + \mathbf{a}.\nabla_{\mathbf{v}} f = Q \qquad (1)$$

Where f indicates the particle distribution function that represents the number of particles moving with velocity $\mathbf{v}$ at position $\mathbf{x}$ at time t. $\mathbf{a}$ represents the acceleration (force per unit mass) and Q is the collision integral, which describe the change in particle distribution function due to collision. $\nabla_{\mathbf{x}}$ and $\nabla_{\mathbf{v}}$ are the gradient with respect to spatial coordinates and velocity respectively.

Equation (1) is an integro-differential equation [10] whose solution is almost an impossible job. The collision integral is simplified using the Bhatnagar-Gross-Krook (BGK) approximation which states that in collision particle distribution functions relax toward their

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equilibrium values at the rate of relaxation time τ .After BGK approximation (1) reads:

$$\frac{\delta f}{\delta t} + \mathbf{v}.\nabla_{\mathbf{x}} f + \mathbf{a}.\nabla_{\mathbf{v}} f = -\frac{1}{\tau}\left(f - f^{eq}\right) \quad (2)$$

Where, f^{eq} is the equilibrium distribution function. To solve (2) is still a very difficult task so it is further simplified by general discretization methods. In the absence of external force $\mathbf{a}=0$, to discretize the velocities a finites set of velocities (nine velocity directions have been considered here , since a D2Q9 model has been used which represents two dimensions and nine velocity components) is used. The distribution function associated with ith velocity is f_i. For a D2Q9 model these velocities are:

$$\mathbf{v}_i = \begin{cases} (0,0) & i = 0 \\ (\pm 1,0),(0,\pm 1) & i = 1\text{—}4 \\ (\pm 1,1),(\pm 1,-1) & i = 5\text{—}8 \end{cases} \quad (3)$$

The space and time are discretized using the usual discretization and applying $\Delta \mathbf{x}_i = \mathbf{v}_i \Delta t$,

$$f_i(\mathbf{x} + \mathbf{v}_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t) = -\frac{\Delta t}{\tau}\left(f_i - f_i^{eq}\right) \quad (4)$$

f_i^{eq} is computed using the following expression:

$$f_i^{eq}\left(\mathbf{x}\right) = w_i \rho \left[1 + 3\frac{\mathbf{v}_i.\mathbf{u}}{c^2} + \frac{9}{2}\frac{\left(\mathbf{v}_i.\mathbf{u}\right)^2}{c^4} - \frac{3}{2}\frac{\mathbf{u}^2}{c^2}\right] \quad (5)$$

Where w_i represent the weights of the lattice. For a D2Q9 lattice, these weights are:

$$w_i = \begin{cases} 4/9 & i = 0 \\ 1/9 & i = 1\text{—}4 \\ 1/36 & i = 5\text{—}8 \end{cases} \quad (6)$$

c is the basic lattice speed and usually c =1 in simple implementations. ρ and $\mathbf{u}$ denote the macroscopic density and fluid velocity respectively.

Since the system used here is composed of artificial particles so the units used have been non-dimensionalized. The dimensions of mass are mu, of length are lu and of time are ts. The dimensions of all other quantities can be obtained using these three basic dimensions.

The macroscopic density ρ is computed as the sum of distribution functions:

$$\rho = \sum_{i=0}^{8} f_i \quad (7)$$

The macroscopic velocity $\mathbf{u}$ is computed as the first moment of particle distribution functions:

$$\mathbf{u} = \frac{1}{\rho}\sum_{i=0}^{8} f_i \mathbf{v}_i \quad (8)$$

Pressure P is calculated by using the following equation of state:

$$P = \rho c_s^{\,2} \quad (9)$$

Where c_s is the speed of sound and for a D2Q9 lattice it is calculated as:

$$c_s = \frac{1}{\sqrt{3}} c \quad (10)$$

The viscosity ν is computed as:

$$\nu = \frac{1}{3}\left(\tau - \frac{1}{2}\right) \quad (11)$$

To achieve physically realistic results, the value of relaxation time τ should be greater than ½ [11]. Relaxation parameter ω is defined as the reciprocal of relaxation time hence for stable results the value of ω should be less than 2.

To model the flow through complex geometries, one simply has to declare that node as solid and apply the bounceback boundary condition there. No extra programming is required.

III. LBM FOR MULTIPHASE FLOW

LBM is a good choice for simulating the multiphase flow. There are various LBM models which can simulate multiphase flow, but the most widely used is Shan and Chen model. The reason for the popularity of Shan and Chen model is its versatility and simplicity. Moreover in this model phase transition takes place spontaneously whereas in other models extra coding is required to incorporate phase transition.

In modeling multiphase flow, an interaction force is introduced between the molecules and automatic phase segregation into dense and light phase occurs when this interaction force exceeds its critical limit. In its implementation, equilibrium distribution function is computed using the equilibrium velocity $\mathbf{u}^{eq}$ rather than fluid velocity:

$$f_i^{eq}\left(\mathbf{x}, t\right) = w_i \rho \left[1 + 3\frac{\mathbf{v}_i.\mathbf{u}^{eq}}{c^2} + \frac{9}{2}\frac{\left(\mathbf{v}_i.\mathbf{u}^{eq}\right)^2}{c^4} - \frac{3}{2}\frac{\mathbf{u}^{eq2}}{c^2}\right] \quad (12)$$

The equilibrium velocity is calculated as:

$$\mathbf{u}^{eq} = \mathbf{u} + \frac{\tau \mathbf{F}}{\rho} \quad (13)$$

Where, $\mathbf{F}$ is the force term introduced between the particles. This interparticle force should be attractive for phase separation. The force term for single component multiphase flow is:

$$\mathbf{F}(\mathbf{x}, t) = -G\ \psi(\mathbf{x}, t)\sum_{i=0}^{8} w_i\ \psi\left(\mathbf{x} + \mathbf{v}_i \Delta t, t\right) \mathbf{v}_i \quad (14)$$

where, G is the interaction strength and it is also known as temperature like parameter and behaves as the inverse of temperature. ψ is the interaction potential between the molecules and w_i are the usual lattice weights. There are various methods to calculate the interaction potential, the most widely used expression is:

$$\psi(\rho) = \psi_0 \exp\left(-\frac{\rho_0}{\rho}\right) \quad (15)$$

Where ψ_0 and ρ_0 are the arbitrary constants and in the present study, the values of ψ_0 and ρ_0 has been chosen as 4 and 200 respectively, because the model behavior with these values has been explored thoroughly[8].

In two phase flow, the pressure is computed using the following non ideal equation of state:

$$P = \frac{\rho}{3} + \frac{G}{6}\psi^2(\rho) \quad (16)$$

The above equation comprises two parts; the first part is same as in single phase flow, whereas, the second part accounts for the non-ideality between the phases. For attractive forces, the value of interaction strength should negative leading to the negative second term in the above expression. This negative term reduces the pressure and hence two phases separate.

The gravity force can be incorporated into this single component multiphase LBM using the same procedure as for the interaction force in (13). The value of gravity is directly substituted into the equilibrium velocity.

IV. RESULTS AND DISCUSSIONS

Poisuelle flow is the simplest flow that can be simulated using LBM. So, it has been simulated here as a test case to check the validity of LBM. Results for flow through complex geometries have also been shown. Then, simulation results for multiphase flow have also been described.

A. *Poisuelle flow*

The steady flow of an incompressible fluid between two parallel plates due to pressure gradient is known poisuelle flow. Its analytical solution provides a parabolic velocity profile with maximum velocity in the middle of the channel and zero velocity at the wall. It has been simulated in LBM using a uniform mesh 30 X 20 lu^2. The value of relaxation parameter, which shows the relaxation rate is 1.85. The length of time is 3000 ts. No slip boundary condition has been applied at the walls and periodic boundary condition in the flow direction. Fig.1 shows the comparison of the analytical results and simulation results using LBM.

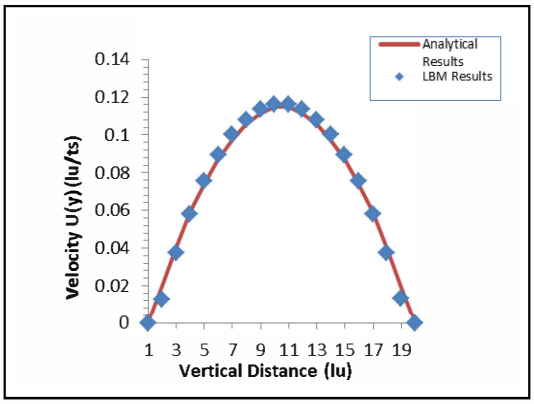

Figure 1. Comparison of LBM and analytical results

It can be seen that both results match quite well. So, LBM can be applied successfully to the poisuelle flow. Slight difference observed at the walls is due to the application of full way bounceback boundary condition which is first order accurate. The remedy is the use of half way bounceback there, since it is second order accurate and leads to better results but at the cost of computation time.

B. *Flow through Complex Geometries*

Flow of oil from its reservoirs is usually through complex geometries resembling porous media. Flow through complex boundaries is difficult to simulate using conventional CFD techniques. In LBM, these complex boundaries are easily incorporated by the bounceback boundary condition. In the code implementation, one simply has to declare it as solid node and the bounceback boundary condition will take care of it.

Figure 2. Comparison of LBM results with analytical solution

Moreover, only those nodes need to be simulated which are active; having direct contact with the fluid. The nodes inside the solids which do not have direct contact with the fluid do not require simulation. They are considered as inactive nodes. Simulation results for such complex geometries are shown in Fig.2. It has been observed that at low velocities, there is no vortex formation but when velocity is increased, then there is vortex shedding behind the largest obstacle. A low pressure zone is formed behind the obstacle due to pressure loss when it strikes with solid. Swirling is produced in this low pressure zone.

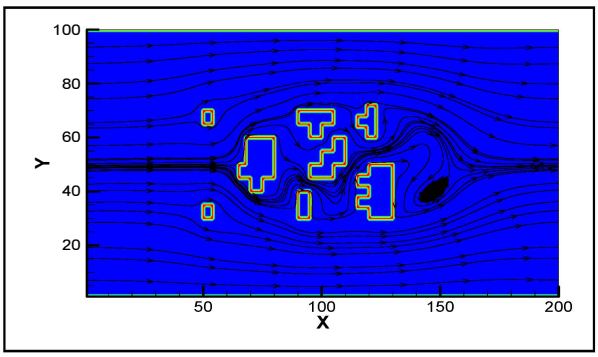

Figure 2. Flow through complex geometries

C. *Multiphase Flow*

Multiphase flow is of great industrial importance. Its simulation is an interesting and challenging task, especially when phase transition is occurring in the flow. The true strength of LBM lies in the simulation of multiphase flow. Phase transition process occurs spontaneously when the interaction force between the particles exceeds its critical limit. Fig.3 demonstrates the simulation results for multiphase flow. Mesh size is 100X100. The value of relaxation parameter is 1.1. Periodic boundary conditions have been applied in all directions. Under the action of interaction force light and dense phases separate from each other and like molecules start coalescing. The red color is indicating the liquid phase and blue is for vapor phase. According to (13), the force is higher on the denser particles, so they move faster

and combine more quickly than lighter ones. With the passage of time, the droplets combine due to the attractive force and finally a single droplet is formed.

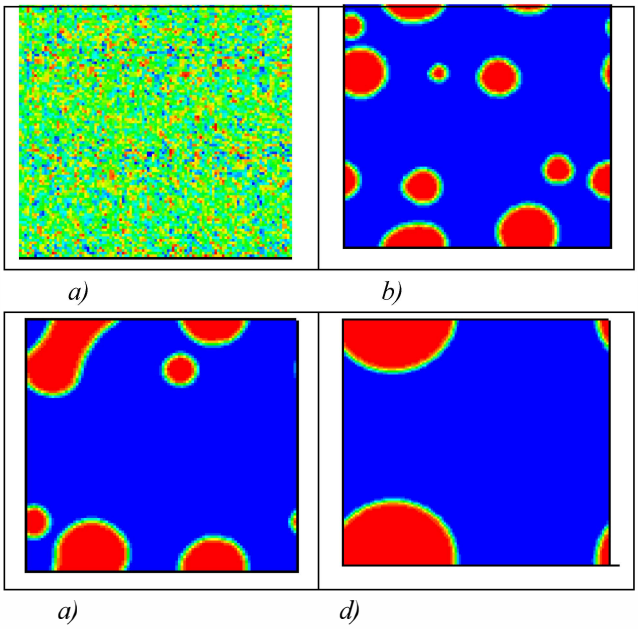

Figure 3. Simulation results for mutiphase flow at time= a)1, b)1000, c)2000 and d)45600 ts

Then vertically downward gravity force has been introduced into the flow. Streamtraces for the single component multiphase flow under the influence of gravity are shown in Fig.4. These streamtraces, which indicate the flow direction are also vertically downward and can be animated on TECPLOT.

The results have been validated by applying laplace law. According to Laplace law, plot of pressure difference between the inside and outside of the droplet and inverse of radius r should be straight line passing through origin. The slope of the plot represents the surface tension σ.

$$\Delta P = \frac{\sigma}{r} \qquad (17)$$

Where, $\Delta P = \left| P_{outside} - P_{inside} \right|$

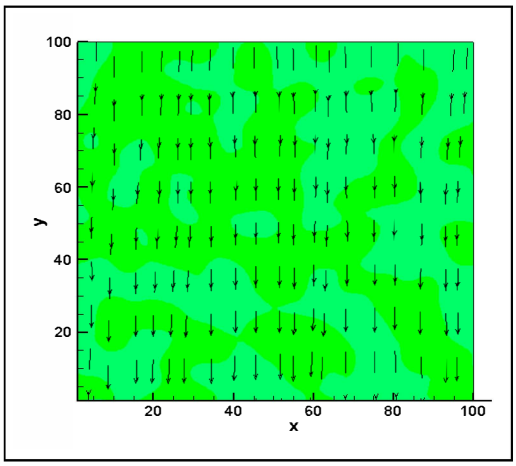

Figure 4. Streamtraces for multiphase flow under the influence of gravity

So, the surface tension σ has been computed by measuring the radii of droplets of various sizes, immersed in their own vapors and their pressure difference. The plot of Pressure difference versus 1/r is shown in Fig.5, which is linear, as stated by Laplace law. The surface tension which is the slope of the straight line comes out to be 34.367 (lu mu/ts^2).

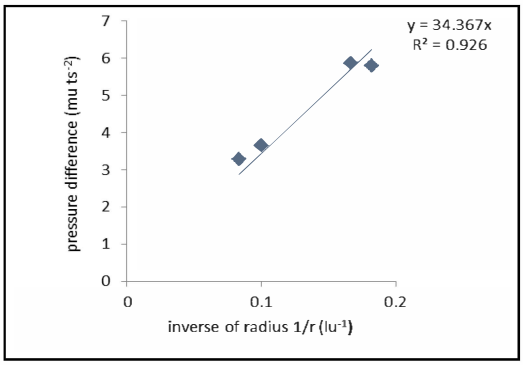

Figure 5. Plot of pressure difference and inverse of radious to compute surface tension.

VI. CONCLUSION

LBM is an accurate and efficient technique emerging as a powerful competitor to traditional CFD techniques. It is easy to understand, program and implement. This paper presents the use of LBM to simulate single phase flow through complex geometries and multiphase flow under the periodic boundary conditions as well as under the action of external gravity force. The simulation results for multiphase flow have been verified by Laplace law. However the use of LBM is limited to low Reynolds numbers.

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