1. Problem setting

In this project, we present a benchmark simulation for segmented flows, which contain discrete droplets and bubbles in micro-channels at small capillary number. In order to test the behavior of LBM and VOF methods, we choose the same setting for the simulation. Cutting of non-wetting phase in T-shaped micro-channel. The 2D problem setting is shown in Figure 1:

As the figure shown, the main channel (filled with wetting phase at beginning) is 1mm wide and 2cm long, with a wetting phase inlet on the left and outlet on the right. The branch channel (filled with non-wetting phase at beginning) is 1mm wide and connects with main channel at 2mm from the wetting phase inlet. The branch channel has a non-wetting phase inlet at the top.

For the boundary conditions with this problem, we set up constant velocity boundaries for both inlets, and we set a constant pressure boundary at the outlet. For simplicity, we apply all non-slip walls for the whole channel.

2. Numerical Method

For the same setting, we use LBM and VOF, two different approaches to solve the problem.

2.1 Volume of fluid (VOF) with OpenFOAM™

In the VOF method, we solve Navier-Stokes equation and continuity equation for each phase simultaneously for the whole flow field. We consider Newtonian, incompressible and immiscible for both phases.

2.1.1 Governing equations

The governing equations can be written as:

$$\nabla \cdot \mathbf{U} = 0$$
\[
\frac{\partial \rho_b U}{\partial t} + \nabla \cdot (\rho_b U U) = -\nabla p + \nabla \cdot \mu_b (\nabla U + \nabla U^T) + \rho_b f + F_s
\]

where \( U \) is the fluid velocity; \( p \) is the pressure; \( f \) is the gravitational force; and \( F_s \) is the volumetric representation of the surface tension. The bulk density \( \rho_b \) and viscosity \( \mu_b \) are averages over two phases:

\[
\rho_b = \rho_w \alpha + \rho_n (1 - \alpha) \\
\mu_b = \mu_w \alpha + \mu_n (1 - \alpha)
\]

where \( \rho_w, \rho_n \) representing density for wetting and non-wetting phases, and \( \mu_w, \mu_n \) are viscosity for wetting and non-wetting phases.

The surface tension is represented as a volumetric force \( F_s \),

\[
F_s = \gamma \kappa (\nabla \alpha)
\]

where \( \kappa = \nabla \cdot (\nabla \alpha / |\nabla \alpha|) \) is the curvature of the interface.

### 2.1.2 Algorithm analysis

In order to solve for the PDE, we discretize the system with 1x1mm size blocks with *blockMesh* in OpenFOAM. In this case, the main channel was discretized into 200x10 blocks and the branch channel was discretized into 10x20 blocks. The discretization plot is shown in Figure 2.

![Figure 2. blockMesh Geometry](image)

Then we specify uniform velocity and zero-gradient pressure at inlets. At outlets, we specify fixed-value pressure and zero-gradient velocity. We also set walls to be non-slip.

### 2.2 Lattice Boltzmann Method (LBM)

LBM is a new approach developed in recent 20 years. In this approach, we treat the fluid with Boltzmann distribution. For the fluid “particle” at certain spatial and temporal location \( (x, t) \), we have a Boltzmann function \( f_{(x,t)}(\vec{x}) \) to describe the probability distribution of this certain fluid “particle” in the flow field. From the Boltzmann function, we can derive lot information, including the density, the velocity and a lot more at \( (x, t) \):

\[
\rho(x, t) = \int_D f_{(x,t)}(\vec{x}) \, dV, (\vec{x} \in D)
\]

\[
\rho u(x, t) = \int_D (\vec{x} - x) f_{(x,t)}(\vec{x}) \, dV, (\vec{x} \in D)
\]

where \( D \) is the flow domain.
2.2.1 The idea of Lattice Boltzmann functions

It is impossible to record complete Boltzmann functions in the simulator. The idea of Lattice Boltzmann is discretizing the flow domain into lattice blocks. For certain position \((x, t)\), which is the center of a certain block, we again discretize Boltzmann function to fit in the blocks in the flow domain. We only choose Boltzmann function from the block itself and surrounding blocks to approximate the entire Boltzmann distribution. For our 2D case, the Boltzmann function we use for every flow domain block includes 9 values in total.

For a multi-component system, we record every component’s Boltzmann function for every lattice block as \(f_{i,\sigma}(x, t)\), where \(i\) is the number of lattice blocks in the flow field, and \(\sigma\) represents the component.

2.2.2 Governing equations (discretized) from LBGK\(^{[2]}\)

Here we set time step as \(\Delta t\). The governing equations for Lattice Boltzmann Method is an explicit evolution equation for the Boltzmann function:

\[
f_{i,\sigma}(x + e_i \Delta t, t + \Delta t) - f_{i,\sigma}(x + e_i \Delta t, t) = -\frac{1}{\tau} [f_{i,\sigma}(x, t) - f_{i,\sigma}^{(eq)}(x, t)]
\]

Where the equilibrium Boltzmann distribution \(f_{i,\sigma}^{(eq)}\) is generated from DnQb\(^{[3]}\) model

\[
f_{i,\sigma}^{(eq)} = \omega_i \rho \left[ 1 + \frac{e_i \cdot u}{c_s^2} + \frac{(e_i \cdot u)^2}{2c_s^4} - \frac{u^2}{2c_s^2} \right]
\]

Where for 2D problem:

\[
e_i = \begin{cases} 
    (0,0)c, i = 5\text{(center)} \\
    \cos \left( \frac{(i-1)\pi}{2} \right), \sin \left( \frac{(i-1)\pi}{2} \right)c, i = 1,3,7,9\text{(corner)} \\
    \sqrt{2} \left[ \cos \left( \frac{(2i-9)\pi}{4} \right), \sin \left( \frac{(2i-9)\pi}{4} \right) \right], i = 2,4,6,8\text{(edge)}
\end{cases}
\]

\[
\omega_i = \begin{cases} 
    \frac{4}{9}, i = 5\text{(center)} \\
    \frac{1}{9}, i = 1,3,7,9\text{(corner)} \\
    \frac{1}{36}, i = 2,4,6,8\text{(edge)}
\end{cases}
\]

\[
c_s^2 = \frac{1}{3}c = \frac{1}{3} \frac{\delta x}{\Delta t}
\]

The relaxation time is related to the kinematic viscosity:

\[
\nu_\sigma = \left( \tau_\sigma - \frac{1}{2} \right) c_s^2 \Delta t
\]

And then we can calculate macroscopic properties from the Boltzmann function:

\[
\rho_\sigma = \sum_i f_{i,\sigma}^{temp}(x, t)
\]

\[
\rho_\sigma u = \sum_i e_i f_{i,\sigma}^{temp}(x, t)
\]
2.2.3 Multicomponent model from Shan-Chen\[3\]

We implement the Shan-Chen attractive or repulsive interaction among components to describe multiphase behavior. If the repulsive interaction is large enough, the components will separate spontaneously to form different phases. And this force can guarantee phase separation and introduce surface-tension effects. This interaction is introduced after we calculate the macroscopic properties of the fluid and we make corrections to the density and velocity.

The interaction potential between component \( \sigma \) and \( \bar{\sigma} \) is:

\[
F_\sigma(x) = -\rho_\sigma(x) \sum_\sigma \left( g_{\sigma\bar{\sigma}} \sum_l \left[ \rho_{\bar{\sigma}}(x + e_l \delta_t) e_l \omega_l \right] \right)
\]

Also in order to describe the contact angle, we introduce interactions between fluid and solid wall:

\[
F_{ads}(x) = -\rho_\sigma(x) \sum_\sigma \left( g_{\sigma\bar{\sigma}} \sum_l \left[ s(x + e_l \delta_t) e_l \omega_l \right] \right)
\]

Then we correct the velocity by (original velocity is \( u_\sigma \)):

\[
\begin{align*}
\text{Original velocity:} & \quad u_\sigma \\
\text{New velocity:} & \quad u^{(eq)}_\sigma \quad \text{where} \quad u^{(eq)}_\sigma = u + \tau_\sigma \delta_t \frac{\bar{F}_\sigma}{\rho_\sigma} \\
\quad \text{and} \quad & \quad u' = \sum_\sigma \frac{\rho_\sigma u_\sigma}{\tau_\sigma} / \sum_\sigma \frac{\rho_\sigma}{\tau_\sigma}
\end{align*}
\]

Where the new velocity of fluid is \( u^{(eq)}_\sigma \).

3. Results and comparison

3.1 T-junction Cutting of oil bubble

We run the OpenFoam and LBM for the same settings, where the two fluids have same kinematic viscosity (\( \nu = 6 \times 10^{-5} m^2/s \)), and the contact angle of oil phase is 45\(^\circ\). We set the initial state which the main channel is filled with wetting phase and the branch channel filled with non-wetting phase. The initial distribution was shown in Figure 1. The following figure 3 shows the initial state for LBM and VOF.

![Figure 3a. Initial setting for LBM](image-url)
If we compare results from both methods, we can observe a similar oil bubble cutting procedure as figure 4 shows. We can see the bubble have very similar size and location at the same time.

Figure 4a. $t = 0.01s$, Left: LBM, Right: VOF

Figure 4b. $t = 0.40s$, Left: LBM, Right: VOF
Figure 4c. $t = 0.80\text{s}$, Left: LBM, Right: VOF

Figure 4d. $t = 1.00\text{s}$, Left: LBM, Right: VOF

Figure 4e. $t = 1.20\text{s}$, Left: LBM, Right: VOF
Figure 4f. $t = 1.30s$, Left: LBM, Right: VOF

Figure 4g. $t = 1.40s$, Left: LBM, Right: VOF

Figure 4h. $t = 1.50s$, Left: LBM, Right: VOF
We can observe that in LBM, the droplet forming time is shorter than VOF, and the bubble size is smaller than VOF. When the droplet is getting off the branch channel, in LBM method, the droplet directly will stick to the bottom wall; while in VOF, the droplet has phase interface diffusion. The problem might because the gridding is not fine enough around the intersection of main and branch channel. Take a finer gridding might improve the behavior in this problem. However, if we just consider the flow behavior of T-junction cutting, both methods describe the problem very good.

Then we compare results for velocity field in Figure 5. Both methods have similar behavior that there is rotational flow at the edge of the bubble.

This behavior can be explained by the conservation of angular momentum. When wetting phase in the main channel flow through, it gives the non-wetting phase droplet a counter-clockwise angular momentum by viscous force. This angular momentum is conserved by non-wetting phase droplet finally developed into a rotational flow.

After the droplet takes off from the intersection, the rotational flow is reduced by friction with channel walls. As Figure 6 shows, the rotational flow is weaker than in figure 5.
4. Conclusion and further research

Our work compared two different numerical simulation methods: Lattice Boltzmann and Volume of Fluid for the same T-junction 2-phase flow simulation. The results already show that both method have very good potential in simulating micro-scale flow regime problems. Since we just start from very simple model for both approach, the simulation behavior can be continued improving by introducing more correction method to the models.

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References: