Lattice Boltzmann Method for Multiphase Flows with High Density and Viscosity Ratios

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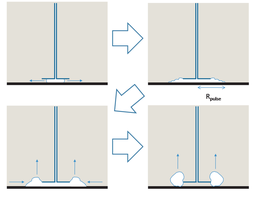
Background

- As a result of atomic weapons production, millions of gallons of radioactive waste was generated and stored in underground tanks at various U.S. Department of Energy sites.
- Department of Energy is currently in the process of transferring the waste from single shell tanks to double shell tanks. Various waste retrieval and processing methods are employed during the transfer of the waste.
- One such method, *pulsed-air mixing*, involves injection of discrete pulses of compressed air or inert gas at the bottom of the tank to produce large bubbles that rise due to buoyancy and mix the waste in the tank as a result of this rising motion.
- Pulsed-air mixers are operated by controlling the pulsing frequency and duration, the sequence of injection plates and gas pressure.
- Understanding the physical nature of the mixing process by injection of bubbles and the effects of the gas release process to the tank environment needs to be studied by considering various waste properties.
- Such an analysis can be made possible by developing a numerical method that can simulate the process of air bubble generation inside tanks filled with liquid.

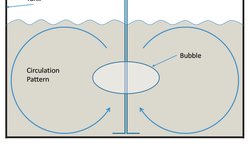
Pulsed-Air Mixing

- The pulsed-air mixing technique uses discrete pulses of air or inert gas to produce large bubbles near the tank floor.
- The bubbles induce mixing as they rise to the surface of the liquid.
- When compressed air is supplied to the underside of the accumulator plate, the growing bubble expels liquid outward from under the plate.
- Bubble growth continues outward beyond the edge of the accumulator plate to a distance of R_{pulse} from the plate center.



Sketch of bubble-growth during Pulsed-air mixing

Pulsed-air mixing array in 1/12-scale tank



Sketch showing mixing pattern induced by the rising bubble.

A pulsed-air mixer in action at the ORNL Gunite and Associated Tanks simulant tank

(*Pulsed -Air Mixer*. Innovative Technology Summary Report. DOE/EM-0462, 1999.)

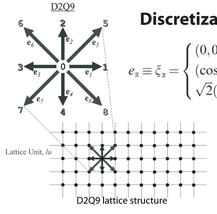
Lattice Boltzmann Method

The Boltzmann equation: kinetic equation that describes the evolution of particle distribution function.

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi}\cdot\nabla f + \mathbf{F}\cdot\nabla_{\xi} f = \Omega_c\,, \qquad \nabla_{\xi} f \approx \nabla_{\xi} f^{eq} = -\frac{\xi - \mathbf{u}}{\rho c_s^2} f^{eq}$$

$$\frac{\partial f_\alpha}{\partial t} + \xi_\alpha\cdot\nabla f_\alpha = \Omega_c + S_{f\alpha}\,, \qquad S_{f\alpha} = \frac{(e_{\alpha i} - u_i)F_i}{\rho c_s^2} f_\alpha^{eq}$$

D2Q9



D2Q9 lattice structure

Discretization process:

$$e_\alpha \equiv \xi_\alpha = \begin{cases} (0,0), & \alpha = 0, \\ (\cos\theta_\alpha, \sin\theta_\alpha)c, & \theta_\alpha = (\alpha-1)\pi/2, \quad \alpha = 1,2,3,4, \\ \sqrt{2}(\cos\theta_\alpha, \sin\theta_\alpha)c, & \theta_\alpha = (\alpha-5)\pi/2 + \pi/4, \quad \alpha = 5,6,7,8. \end{cases}$$

Single-phase lattice Boltzmann equation:

$$f_\alpha(\mathbf{x} + \mathbf{e}_\alpha\delta_t, t + \delta_t) - f_\alpha(\mathbf{x}, t) = \boldsymbol{\Omega}_{coll}\delta_t$$

f : The single-particle distribution function the phase space (x_i, ξ_i)
$\boldsymbol{\xi}$: The microscopic velocity
$\mathbf{F}$: External body force
λ : The relaxation time due to collision.
f^{eq} : Maxwell-Boltzmann distribution function
c_s : speed of sound

[1] Collision Step

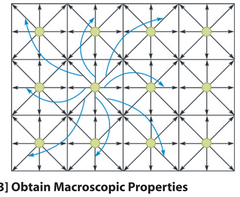
$$\Omega_c = -\left(\frac{f_\alpha - f_\alpha^{eq}}{\lambda}\right) \qquad \tau = \frac{\lambda}{\delta_t}$$

Bhatnagar-Gross-Krook (BGK) collision operator

$$f_\alpha^{eq} = w_\alpha\rho\left[1 + \frac{e_{\alpha i}u_i}{c_s^2} + \frac{(e_{\alpha i}e_{\alpha j} - c_s^2\delta_{ij})u_i u_j}{2c_s^4}\right]$$

$$w_\alpha = \begin{cases} 4/9, & \alpha = 0, \\ 1/9, & \alpha = 1,2,3,4, \\ 1/36, & \alpha = 5,6,7,8. \end{cases}$$

[2] Streaming Step



[3] Obtain Macroscopic Properties

$$\rho = \sum_{\alpha=0}^{8} f_\alpha \qquad \mathbf{u} = \frac{1}{\rho}\sum_{\alpha=0}^{8} f_\alpha \mathbf{e}_\alpha$$

Multiphase Lattice Boltzmann Method

Objective: To use the multiphase lattice Boltzmann method for flows with high density and viscosity ratios. To achieve this, a two-distribution function LBM is used (Lee and Lin (2005)).

LBE for order parameter

$$\frac{\partial f_\alpha}{\partial t} + e_{\alpha i}\frac{\partial f_\alpha}{\partial x_i} = -\frac{1}{\lambda}\left(f_\alpha - f_\alpha^{eq}\right) + \frac{(e_{\alpha i} - u_i)\left[\partial_i\rho c_s^2 - \rho\partial_i\left(\varphi - \kappa\partial_j^2\rho\right)\right]}{c_s^2}\Gamma_\alpha(\mathbf{u}) \qquad \Gamma_\alpha(\mathbf{u}) = \frac{f_\alpha^{eq}}{\rho}$$

κ : the surface tension parameter
σ : surface tension

$$\sigma = \kappa\int\left(\frac{\partial\rho}{\partial r}\right)^2 \mathrm{d}r$$

$E_f(\rho)$: Excess free energy at the interface over the bulk free energies is obtained from an equation of state:

$$E_f(\rho) \approx \beta(\rho - \rho_g^{sat})^2(\rho - \rho_l^{sat})^2$$

$$\rho(z) = \frac{\rho_l^{sat} + \rho_g^{sat}}{2} - \frac{\rho_l^{sat} - \rho_g^{sat}}{2}\tanh\left(\frac{2z}{D}\right)$$

$$D = \frac{4}{(\rho_l^{sat} - \rho_g^{sat})}\sqrt{\frac{\kappa}{2\beta}}$$

$$\sigma = \frac{(\rho_l^{sat} - \rho_g^{sat})^3}{6}\sqrt{2\kappa\beta}.$$

β : consant
ρ_g^{sat} : gas phase saturation density
ρ_l^{sat} : liquid phase saturation density
z : spatial location normal to the interface
D : interface thickness

LBE for pressure and momentum

$$\frac{Dg_\alpha}{Dt} = -\frac{1}{\lambda}(g_\alpha - g_\alpha^{eq}) + \frac{(e_{\alpha i} - u_i)\partial_i(\rho c_s^2 - p)}{c_s^2}\left[\Gamma_\alpha(\mathbf{u}) - \Gamma_\alpha(0)\right] + \frac{(e_{\alpha i} - u_i)\left[\kappa\partial_i(\partial_k\rho\partial_k\rho) - \kappa\partial_j(\partial_i\rho\partial_j\rho)\right]}{c_s^2}\Gamma_\alpha(\mathbf{u})$$

Obtaining hydrodynamic variables from f_α results in numerical instabilities due to the steep density gradients involved in the computation of the source term. A seperate distribution function g is used to compute pressure and momentum.

$$g_\alpha = f_\alpha + \left(\frac{p}{c_s^2} - \rho\right)\Gamma_\alpha(0) \qquad p = P - \kappa\rho\frac{\partial^2\rho}{\partial x_k\partial x_k} + \frac{\kappa}{2}\frac{\partial\rho}{\partial x_k}\frac{\partial\rho}{\partial x_{k\beta}}$$

$$g_\alpha^{eq} = t_\alpha\left[\frac{p}{c_s^2} + \rho\left(\frac{e_{\alpha i}u_i}{c_s^2} + \frac{(e_{\alpha i}e_{\alpha j} - c_s^2\delta_{ij})u_i u_j}{2c_s^4}\right)\right].$$

$$\rho = \sum_\alpha \bar{f}_\alpha,$$

$$\rho u_i = \sum_\alpha \mathbf{e}_{\alpha i}\bar{g}_\alpha + \frac{\delta t}{2}\kappa\left[\frac{\partial}{\partial x_i}\left(\frac{\partial\rho}{\partial x_k}\frac{\partial\rho}{\partial x_k}\right) - \frac{\partial}{\partial x_j}\left(\frac{\partial\rho}{\partial x_i}\frac{\partial\rho}{\partial x_j}\right)\right]$$

$$p = \sum_\alpha \bar{g}_\alpha + \frac{\delta t}{2}u_i\frac{\partial\rho c_s^2}{\partial x_i}.$$

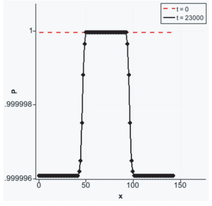
(*Lee T, Lin CL*. A stable discretization of the lattice Boltzmann equation for simulation of incompressible two-phase flows at high density ratio. J Comput Phys, 206:16, 2005)

Static Bubbles

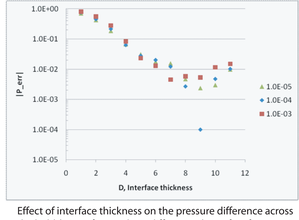
The LBM was tested for static bubbles with a density ratio of 1000 and a viscosity ratio of 100.

Laplace's law for surface tension was used to verify the results for the pressure difference:

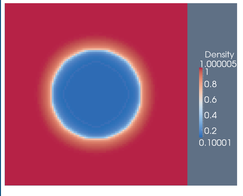
$\Delta P = \sigma/R$



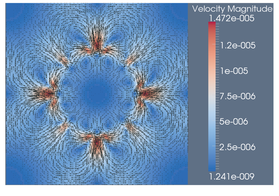
Initial and final pressure distribution across the bubble cross section.



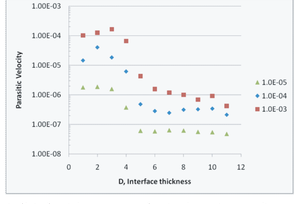
Effect of interface thickness on the pressure difference across the bubble interface at three different values of surface tension



Initial density distribution of the bubble.



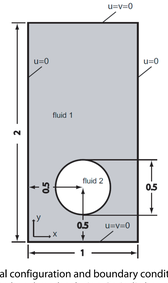
Spurious velocity field around the bubble.



Effect of interface thickness and surface tension on the magnitude of maximum parasitic velocity in the vicinity of the bubble interface.

Dynamic Bubbles

The multiphase LBM was used to simulate single bubbles rising in a fluid column. The results for two test cases were found to be in agreement with a benchmark solution (Hysing, 2008).



Initial configuration and boundary conditions in the benchmark solution. Periodic boundaries were applied in the LBM simulation.

$$Eo = \frac{g(\rho_H - \rho_L)d^2}{\sigma}$$

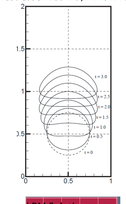
$$Re = \frac{\rho_H V_T d}{\mu_H}$$

$$M = \frac{g(\rho_H - \rho_L)\mu_H^4}{\rho_H^2\sigma^3}$$

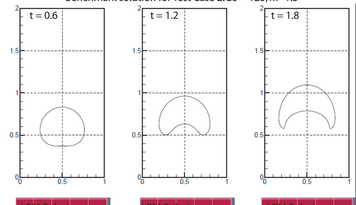
Test Case	Re	Eo	ρ_1/ρ_2	μ_1/μ_2
1	35	9	10	10
2	35	125	1000	100

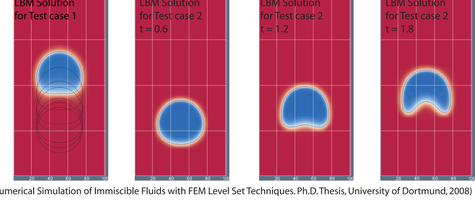
Physical parameters and dimensionless numbers defining the benchmark test cases.

Benchmark Solution for Test Case 1: Eo = 9, M= 6 x 10^{-4}



Benchmark solution for Test Case 2: Eo = 125, M=1.3





(*Hysing, S.R.*, Numerical Simulation of Immiscible Fluids with FEM Level Set Techniques. Ph.D. Thesis, University of Dortmund, 2008)