

DPD Simulation of Multiphase Flow at Small Scales

Mou-Bin Liu^{1,2}

¹ Institute of Mechanics
Chinese Academy of Sciences
Beijing 100190, China
e-mail: liumoubin@imech.ac.cn

Jian-Zhong Chang², Han-Tao Liu²

² School of Mechatronic Engineering,
North University of China
Taiyuan, Shanxi 030051, China
e-mail: jianzhong.chang@gmail.com, liuht@nuc.edu.cn

Abstract—Small scale multiphase fluid motion is fundamentally important for applications in environmental, biological and chemical engineering as well as many other areas. Due to the existence of complex geometries, arbitrarily moving interfaces, and large density and viscosity contrast, simulation of small scale multiphase flows has been a formidable task for traditional grid-based numerical methods. This paper presents the application of a meso-scale, Lagrangian particle method, dissipative particle dynamics (DPD), for simulating multiphase fluid flows. For multiple component multiphase flows, with properly selected coefficients, the conventional DPD model can be directly used. For single component multiphase flows, the conservative weight function describing DPD particle-particle interactions has to be modified to model the existing liquid-gas phases. The effectiveness of the DPD model in simulating multiphase flows has been demonstrated by two numerical examples of two-component two phase flow, and one-component two phase flow.

Keywords- *dissipative particle dynamics, multiphase flow, meso-scale, micro-scale*

I. INTRODUCTION

Multiphase fluid motion at small scales (meso-scale or/and micro-scale) can be frequently found in environmental, biological and chemical engineering as well as many other areas. Typical examples include saturated and unsaturated water flow in pore-scale subsurface fractures and porous media [1], ink-jet printing, DNA and protein micro- or nano-arraying, and fabrication of particles and capsules for controlled release of medicines [2, 3]. Characterization of multiphase flows at small scales has increasingly becoming a very important topic since the associated flow behavior is very different from what observed in daily life. Except for features similar to those in continuum scale flows such as moving interfaces and large flow deformation, small scale fluid flows usually involve small or ignorable inertial force, but dominant viscous, electro-kinetic and surface effects especially when the surface-to-volume ratio increases. Analytical or semi-analytical solutions for small scale multiphase flows are generally limited to a very few simple cases, whereas experimental studies are usually expensive and also difficult to implement. Simulation of small scale multiphase flows is not easy due to the associated complex features including movable boundaries (free surfaces and moving interfaces), large surface-to-volume ratio, and

phenomena due to small scale physics. These requirements together with small scale phenomena and complex boundaries (fluid-fluid-solid contact line dynamics and fluid-fluid interface dynamics) present severe challenges to conventional grid-based numerical methods which require special algorithms to treat and track the interface between different phases [4, 5]. Molecular dynamics (MD) [6], as a fundamental way of obtaining a good understanding of the behavior of small scale multiphase flows, is computationally expensive, even for modern supercomputers. Therefore numerical studies with reliable models are needed to develop a better understanding of the temporal and spatial dynamics of multiphase flows at small scales.

Dissipative particle dynamics [7] is a relatively new meso-scale modeling technique that has been used to simulate the behavior of complex fluids, mainly by the computational physics community. In DPD simulations, the particles represent a small cluster of atoms or molecules and the particle-particle interactions are much softer than the particle-particle interactions used in typical molecular dynamics simulations [6]. Therefore it is feasible to take much larger particle size and much larger time step, and DPD simulations are much more efficient than MD simulations for the purpose of simulating macroscopic hydrodynamics. DPD can be used to simulate complex fluid systems on physically interesting and important length and time scales, and it rigorously conserves both the number of particles (equivalently, the total mass) and the total momentum of the system [8, 9]. Another advantage of DPD simulations is that DPD is a Lagrangian method, the solid/fluid interface and fluid/fluid interface move with the fluid particles so there is no need to track the interface explicitly. The meso-scale feature together with Lagrangian nature makes DPD method a suitable choice for simulating small scale multiphase fluid flow.

II. DISSIPATIVE PARTICLE DYNAMICS

A. Basic concept

In DPD simulations, a complex system can be simulated using a set of interacting particles. A particle represents a cluster of molecules that interact via conservative (non-dissipative), dissipative and fluctuating forces. A longer time steps combined with a larger particle size makes DPD much more practical to simulate hydrodynamics than MD. DPD is

particularly promising for the simulation of complex liquids, such as polymer suspensions, liquids with interfaces, colloids and gels. Because of the symmetry of the interactions between the particles, DPD rigorously conserves the total momentum of the system, and because the particle-particle interactions depend only on relative positions and velocities, the resulting model fluids are Galilean invariant. Mass is conserved because the same mass is associated with each of the particles, and the number of particles does not change.

In a DPD model, the time evolution for a certain particle, i , is given by the following equation of motion

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i, \quad \frac{d\mathbf{v}_i}{dt} = \mathbf{f}_i = \mathbf{f}_i^{int} + \mathbf{f}_i^{ext}, \quad (1)$$

where \mathbf{r}_i and \mathbf{v}_i are the position and velocity vectors of particle i , \mathbf{f}_i^{ext} is the external force including the effects of gravity, and \mathbf{f}_i^{int} is the inter-particle force acting on particle i . The particle-particle interaction is usually assumed to be pairwise additive and consist of three parts: a conservative (non dissipative) force, \mathbf{F}_{ij}^C , a dissipative force, \mathbf{F}_{ij}^D , and a random force, \mathbf{F}_{ij}^R , i.e. $\mathbf{f}_i^{int} = \sum_{j \neq i} \mathbf{F}_{ij} = \sum_{j \neq i} \mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R$. \mathbf{F}_{ij} is the inter-particle interaction force exerted on particle i by particle j , which is equal to \mathbf{F}_{ji} in magnitude and opposite in direction. This symmetry of the interactions ensures that momentum is rigorously conserved. The pairwise particle interactions have a finite cutoff distance, r_c , which is usually taken as the unit of length in DPD models.

The dissipative force \mathbf{F}_{ij}^D represents the effects of viscosity, and is given by $\mathbf{F}_{ij}^D = -\gamma w^D(r_{ij}) \left(\hat{\mathbf{r}}_{ij} \cdot \mathbf{v}_{ij} \right) \hat{\mathbf{r}}_{ij}$, where γ is a coefficient, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $r = r_{ij} = |\mathbf{r}_{ij}|$, $\hat{\mathbf{r}}_{ij} = \mathbf{r}_{ij} / r_{ij}$, $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ and $w^D(r_{ij})$ is the dissipation weight function. The random force \mathbf{F}_{ij}^R represents the effects of thermal fluctuations, and is given by $\mathbf{F}_{ij}^R = \sigma w^R(r_{ij}) \xi_{ij} \hat{\mathbf{r}}_{ij}$, where σ is a coefficient, $w^R(r_{ij})$ is the fluctuation weight function, and ξ_{ij} is a random variable. The fluctuation-dissipation relationship [10] requires

$$w^D(r) = \left[w^R(r) \right]^2 \quad (2)$$

and

$$\gamma = \frac{\sigma^2}{2k_B T}, \quad (3)$$

where k_B is the Boltzmann constant and T is the temperature. One straightforward choice for the dissipative and random weight functions is

$$w^D(r) = \left[w^R(r) \right]^2 = (1-r)^2, \quad r < 1. \quad (4)$$

B. Conservative force weight function

The conservative force, \mathbf{F}_{ij}^C , is a “soft” interaction acting along the line of particle centres, and has the form $\mathbf{F}_{ij}^C = a_{ij} w^C(r) \hat{\mathbf{r}}_{ij}$, where a_{ij} is the magnitude of the repulsive interaction strength between particles i and j . $w^C(r_{ij})$ is the weight function for the conservative force. In conventional DPD implementations, a conservative force weighting function in a simple form of $w^C(r) = 1-r$ has been widely used for problems with single phase or multiple components in a confined domain or a domain with periodic boundary conditions. Because the fluid generated by DPD simulations with this purely repulsive conservative force is a gas, it cannot be used to simulate the flow of liquids with free surfaces, the behavior of bubbly liquids, droplet dynamics and other important multiphase fluid flow processes. Including a long-range attractive component in $w^C(r)$ is necessary for problems with co-existing liquid-gas phases. One possible approach is to combine the commonly used smoothed particle hydrodynamics (SPH) [1, 11] cubic spline smoothing functions $W(r, r_c)$ with different interaction strengths A and B , and different cutoff distances r_{c1} and r_{c2} , multiplied by an interaction strength coefficient a to construct a new particle-particle interaction potential $U(r)$ as follows

$$U(r) = a(AW(r, r_{c1}) - BW(r, r_{c2})). \quad (5)$$

The conservative force weight function w^C can be derived from the interaction potential as

$$w^C = -U'(r) = -\left(AW_1'(r, r_{c1}) - BW_2'(r, r_{c2}) \right). \quad (6)$$

The constructed interaction potential function $U(r)$ consists of short-range repulsive and large range attractive interactions (when $A > B$, and $r_{c1} < r_{c2}$) and allows the behavior of gases, liquids, solids and multiphase systems to be simulated. A certain set of parameters A, B, r_{c1} and r_{c2} in equation (5) determines the shape of the particle-particle interaction potential which describes the property of the corresponding fluid. The magnitude of the conservative force weight function and the location of the transition point from repulsion to attraction should be easily adjustable to

allow the behavior of different fluids to be simulated. More detailed discussions on the construction of DPD interaction potentials with long-distance attraction and short-range repulsion can be found in [12].

III. NUMERICAL EXAMPLES

The effectiveness of DPD models in simulating single phase fluid flow has already been showcased with applications in different areas [13, 14]. In this section, we will demonstrate the application of the DPD method for multiphase fluid flow at small scales.

A. Two-component two-phase flow

In a DPD model, the strength coefficient (a_{ij}) of the conservative force describes the behavior of the interaction between particles i and j , which can be different for particles from different media. For a system with co-existing component P and component Q , there exists three kind of interactions 1) interaction between particles from component P with a strength coefficient a_{PP} , 2) interaction between particles from component Q with a strength coefficient a_{QQ} , and 3) interaction between particles from component P and component Q with a strength coefficient a_{PQ} . When $a_{PP} < a_{PQ}$ and $a_{QQ} < a_{PQ}$, component P and component Q are immiscible. If all the particles are initially mixed together, particles from component P can be separated with particles from component Q , and the particle interaction leads to phase separation. If particles from each component are initially separated, it is possible to drive the particles from one component with the motion of particles from the other component.

The first numerical example is a two-component two-phase flow problem, which can be frequently found in daily life. One typical example in enhanced oil recovery (EOR) is to use water to drive and recover oil. The computational geometry of the problem is a channel with a middle contraction section (Fig. 1). The size of the computational domain is $90 \times 3 \times 47$ in the x , y and z direction. The coefficients used in the DPD model were $\sigma = 3.0$ and $k_b T = 1.0$ ($\gamma = 4.5$). The conventional conservative weight function is used for this example. In DPD simulations, the effects of solid walls are usually simulated by using fixed particles to represent the solid matrix near the solid-fluid interface [15]. In this example, the upper and lower channel walls were represented by 2881 frozen wall particles. The channel was initially saturated with equilibrated particles from component Q with a number density of 4. Particles from component P were then injected with an injection rate of 200 particles per 100 steps along the first two layers of lattice to drive the particles from component Q . The interaction strength coefficients between the fluid particles was $a_{PP} = a_{QQ} = 18.75$, $a_{PQ} = 25$, $a_{PW} = 37.5$, $a_{QW} = 18.75$, where the subscript W stands for wall particles. The gravitational force is 0.03 along the positive horizontal direction. A modified velocity-Verlet time integration

algorithm was used for time integration with a time step of 0.02 [9]. Fig. 1 shows the snapshots of two-component two-phase fluid flow at different time steps. It can be seen that with the injection of the particles from component P , particles from component Q move along positive horizontal direction. The motion of component P exhibits non-wetting behavior due to a large strength coefficient a_{PW} . With the forward movement of component P , and component Q driven by component P , some particles from component Q were entrapped at the left upper and lower corner near the contraction section. Using other different strength coefficients can lead to different flow driving behavior.

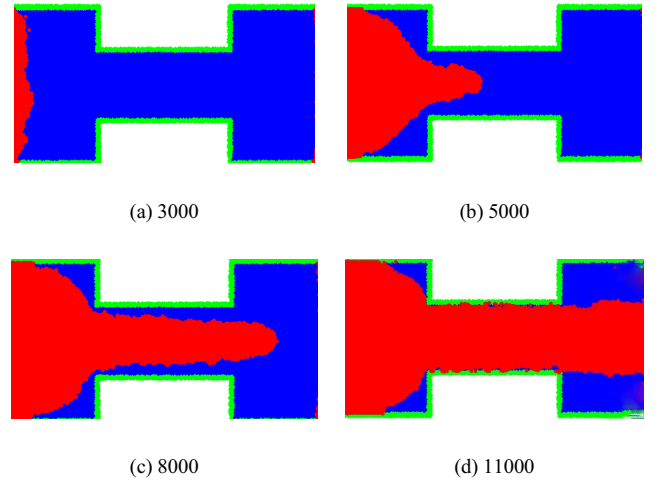


Figure 1. Snapshots of the simulation of two-component two-phase fluid flow at different time steps.

B. Single-component Two-phase Flow

The second example is a single component two phase flow problem in which liquid phase and vapor or gas phase exist. There are very few literature discussing multiphase problems with co-existing liquid-gas phases. One reason is that there lacks a suitable model to describe the behavior of co-existing liquid-gas phases. In this example, the conservative weight function discussed early was used, and the corresponding interaction potential was constructed as $U(r) = a_f (2W_1(r, 0.8) - W_2(r, 1.0))$. It is clear that the interaction potential function is associated with long-distance attraction and short-range repulsion. The strength coefficient between flow DPD particles, a_f , is 18.75, and the strength coefficient between flow and wall DPD particles, a_w , is $5a_f$. The problem domain is a self-affine fracture of $32 \times 3 \times 64$ in the x , y and z direction while particles were injected at an injection rate of 100 particles per 100 steps from the top entrance of the fracture. Other parameters are similar to those in the above example. Fig. 2 shows the snapshots of the fluid motion in the self-affine fracture. The injected fluid particles moved downward, through the self-affine fracture,

as the density of the injected particles and the concomitant pressure increased.

It can be observed that a few particles evaporated from the bulk fluid and the flow was a two-phase flow with co-existing liquid-gas phases. The particles near the fracture walls moved into the fracture faster than those far from the walls, and the fluid exhibited a strong wetting behavior with a small contact angle. The contact angle varied with position and time due to the dynamic balance between viscous, capillary, and gravitational forces. It is expected that the unsaturated fluid may move through localized preferential pathways in a complex fracture network, and this has been observed in subsurface multiphase flows [16].

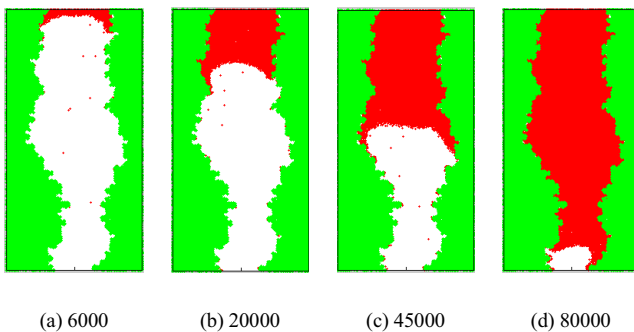


Figure 2. Snapshots of the simulation of two-component two-phase fluid flow at different time steps.

IV. CONCLUDING REMARKS

This paper presents the application of DPD models for simulating multiphase flows. The conventional DPD model can be directly used to simulate multiple-component multiphase fluid motion with properly selected interaction coefficients. Hence it is possible to model fluid flow driving by another immiscible component, and varying interaction coefficients can exhibit different flow driving behaviors. For single component multiphase flows, it is necessary to use conservative particle-particle interactions that combine short-range repulsive and long-range attractive interactions to simulate gases, liquids, solids and multiphase systems, depending on the average particle density, the temperature and the details of the particle-particle interactions. The interaction strength between the fluid particles, and between the fluid and wall particles are closely related to the wetting behaviour and the contact angles. The advancing and receding contact angles can vary spatially and temporally,

depending on the dynamic balance of viscous, capillary and gravitational forces.

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REFERENCES

- [1] M. B. Liu, G. R. Liu and Z. Zong, "An overview on smoothed particle hydrodynamics," *Int. J. Comput. Meth.*, vol. 5 (1), pp. 135-188, 2008.
- [2] G. E. Karniadakis, A. Beskok and A. Aluru, *Microflows and nanoflows: Fundamentals and simulation*, Springer, 2005.
- [3] J. Berthier and P. Silberzan, *Microfluidics for biotechnology*, Artech House, 2006.
- [4] C. W. Hirt and B. D. Nichols, "Volume of fluid/vof/ method for the dynamics of free boundaries," *J. Comput. Phys.*, vol. 39 (1), pp. 201-225, 1981.
- [5] M. Sussman, P. Smereka and S. Osher, "A level set approach for computing solutions to incompressible two-phase flow," *J. Comput. Phys.*, vol. 114 (1), pp. 146-159, 1994.
- [6] D. C. Rapaport, *The art of molecular dynamics simulation*, Cambridge University Press, 2004.
- [7] P. J. Hoogerbrugge and J. Koelman, "Simulating microscopic hydrodynamic phenomena with dissipative particle dynamics," *Europhys. Lett.*, vol. 19, pp. 155, 1992.
- [8] C. Marsh, *Theoretical aspects of dissipative particle dynamics*, University of Oxford, 1998.
- [9] R. D. Groot, "Dissipative particle dynamics: Bridging the gap between atomistic and mesoscopic simulation," *J. Chem. Phys.*, vol. 107 (11), pp. 4423, 1997.
- [10] P. Espanol and P. Warren, "Statistical mechanics of dissipative particle dynamics," *Europhys. Lett.*, vol. 30 (4), pp. 191-196, 1995.
- [11] G. R. Liu and M. B. Liu, *Smoothed particle hydrodynamics: A meshfree particle method*, World Scientific, 2003.
- [12] M. B. Liu, P. Meakin and H. Huang, "Dissipative particle dynamics with attractive and repulsive particle-particle interactions," *Phys. Fluids*, vol. 18 (1), pp. 017101, 2006.
- [13] S. Chen, N. Phan-Thien, B. C. Khoo and X. J. Fan, "Flow around spheres by dissipative particle dynamics," *Phys. Fluids*, vol. 18 (10), 103605, DOI: 10.1063/1.2360421, 2006.
- [14] X. J. Fan, N. Phan-Thien, S. Chen, X. H. Wu and T. Y. Ng, "Simulating flow of DNA suspension using dissipative particle dynamics," *Phys. Fluids*, vol. 18 (6), 063102, DOI: 10.1063/1.2206595, 2006.
- [15] M. B. Liu, P. Meakin and H. Huang, "Dissipative particle dynamics simulation of pore-scale flow," *Water Resour. Res.*, vol. 43, W04411, DOI:10.1029/2006WR004856, 2007.
- [16] H. Huang, P. Meakin and M. B. Liu, "Computer simulation of two-phase immiscible fluid motion in unsaturated complex fractures using a volume of fluid method," *Water Resour. Res.*, vol. 41, W12413, DOI:10.1029/2005WR004204, 2005.