Numerical simulation of coalescence and break-up of drops in shear flow based on the meshless localized radial basis function method

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Abstract. In the present paper, the meshless localized radial basis function (RBF) is proposed for simulating of two-phase incompressible viscous flow. Due to the velocity of the shear flow is very low, the fluid can modeled by Stokes equations. For more convenience the primitive variables, i.e., pressure and velocity components of the Stokes equations are transformed into stream function formulation. The interface of the fluid system is modeled by using Cahn-Hilliard equation. The spatial terms of the governing equations are discretized numerically by using the RBF method. The temporal term is integrated by using fully implicit Euler method. The nonlinear terms of Cahn-Hilliard equation is linearized using the Picard iteration. The proposed method is applied to simulate coalescence and break-up of drops in shear flow. The numerical results show that the deformation of the interface can be modeled without any difficulties.

Introduction

The immiscible multiphase fluid flow problems, such as emulsions and polymer blends, have received much attention. The problems encountered in numerous engineering applications including foods processing, pharmaceutical, chemical and petroleum industries. Understanding the process of droplets of the disperse phase is needed to be improved. This is a challenging problem due to the droplets are deformed, broken-up and coalesced. Experimental and numerical modeling studies [1] have been conducted to providing the better understanding of the behavior of the droplet mechanism. Due to rapid development of digital computers, numerical modeling gained its popularity. The difficulty of the numerical modeling of the droplet mechanism is laid on the interface that separating the deforming disperse phase with the continuous phase must be captured accurately.

Recently, many numerical methods have been developed for modeling the immiscible multiphase flow. Those methods are the front tracking method [2-4], the volume-of-fluid (VOF) method [5,6], level set (LS) method [7–10], Lattice Boltzmann (LB) method [11,12] and the phase field method [13–20].
The front tracking uses the Eulerian grid for the fluid flow and Lagrangian to track the interface, but communication between the Lagrangian and the Eulerian is difficult to handle. In the VOF method, the interface is reconstructed in each grid cell using volume fraction function, which is equal to the volume of one of the fluids. The volume fraction function is advected by flow field and can be modeled using transport equation to track the interface. The curvatures and the normal of the interface are hard to obtain due to discontinuity of the volume fraction function. The LS method uses the level set function to capture the interface. The behavior of the interfacial dynamics can be handled easily using this method, but the mass conservation is worse than VOF. In the last decades the Lattice Boltzmann is popular numerical methods for simulating multiphase flow problems. It is based on simplified Boltzmann equation instead Navier-Stokes equations. The LB method is robust, simple and well suited for parallel implementation. Unfortunately, the LB method needs more memory consumptions than conventional CFD methods, which are based on Navier-Stokes equations. The higher temporal numerical integration is difficult to be implemented in LB method. In the phase field approach, the thickness interface is assumed finite and described by molecular force balance between the fluid phases. The interfacial dynamic behavior can be modeled using Cahn-Hilliard or Allen-Cahn equation, meanwhile the flow field is modeled using Navier-Stokes equations. Using this approach, the mass conservation can be well maintained and the drastic interface changes can be handled easily.

Budiana et al. [19] developed meshless localized radial basis function (RBF) method combined with domain decomposition method (DDM) to solve the two-phase fluid flow, using the Rayleigh-Taylor instability as the example. They used the Cahn-Hilliard equation to capture the interface. Here, we are motivated to extend our previous studies about development the meshless method for solving fluid flow problem [21–25], and in this paper, we propose the RBF method for simulating of coalescence and break-up of drops in shear flow. The flow field is modeling using Stokes equation due to low velocities, therefore, the inertia forces can be neglected and the interface dynamics is modeled using Cahn-Hilliard equation.

**Governing equations**

The governing equations of the multiphase flow problem consist of Stokes Equation in stream function formulation, and Cahn-Hilliard equations in non-dimensionalized form [20]:

**Stokes Equation:**

\[
\nabla^2 \psi = \frac{1}{Ca} \nabla \times \mu \nabla c \\
\]

\[
\psi = \frac{\partial \psi}{\partial y} \\
\]

\[
\nu = -\frac{\partial \psi}{\partial x} 
\]

where \( \psi \) is the stream function, \((u, v)\) is the velocity vector, \( Ca \) is the capillary number and \( C \) is the Cahn number.

**Cahn-Hilliard equations:**

\[
\frac{\partial c}{\partial t} + \frac{\partial uc}{\partial x} + \frac{\partial vc}{\partial y} = \frac{1}{Pe} \left( \frac{\partial^2 \mu}{\partial x^2} + \frac{\partial^2 \mu}{\partial y^2} \right) \\
\mu = c^3 - c - C^2 \left( \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right)
\]
The Equation 2 is determined into two second order differential equations:

\[-\left( \frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2} \right) = \Box \]  
\[-\left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) = \omega \]  

(3a)  
(3b)

Where \( \Box = -\frac{1}{Ca} \frac{1}{c} \mu \nabla c \), \( c \) is the concentration (mass fraction of one of the two fluid phases), \( \mu \) the chemical potential and \( \omega \) is the vorticity and the \( \mu \nabla c \) term denotes the surface tension.

The numerical method

In this paper, the RBF method developed by Sarra [26], is employed for solving the problem numerically. The spatial domain is discretized with a set of \( N \) distinct nodes \( x = \{x_1, \ldots, x_N\} \), called as centers. At each of the nodes, the interpolant and spatial partial derivatives are approximated using multiquadric (MQ) RBF as the basis function:

\[ \varphi(r, \varepsilon) = \sqrt{1 + \varepsilon^2 r^2} \]  

(4)

where \( \varepsilon \) is the shape parameter and \( r \) is the Euclidian distance. The local RBF interpolant for any smooth function \( f(x) \) can be constructed as follows:

\[ f(x_i) = \sum_{j=1}^{n} \alpha_j \varphi(r, \varepsilon) \]  

(5a)

\[ r = \sqrt{x_i^2 + y_i^2} \]  

(5b)

where \( \alpha \) is a vector of expansion coefficients, and \( n \) is the number of the surrounding nodes plus the center. If Eq. (11) is written in a vector-matrix notation, we have \( N \times N \) linear systems to be solved for the expansion coefficients. The matrix \( B \) is called the interpolation matrix.

\[ B \alpha = f \]  

(6)

The matrix \( B \) is used to obtain the spatial derivative operator for the center node \( x_j \), the \( D_x \) operator of partial derivative a function with respect of \( x \) is taken as example:

\[ D_x = B^{-1} H_x \]  

(7)

where matrix \( H_x \) is an \( N \times N \) linear systems with entries:

\[ \Box_{ij} = \frac{\partial}{\partial x} \varphi \left( \|x_i - x_j\|_2 \right) \]  

(8)

By using the operator \( D_x \), the partial derivative a function with respect of \( x \) can be calculated as follows:

\[ \frac{\partial f}{\partial x} = D_x f \]  

(9)

The rest of the partial derivative operators \( (D_y, D_{xx}, D_{yy}) \) are obtained with the same way.
Discretization the governing equation in space using local RBF and implicit Euler method described as follows:

\[
\frac{c^{n+1} - c^n}{\Delta t} + D_x u^n c^{n+1} + D_y v^n c^{n+1} - \frac{1}{Pe} (D_{xx} \mu^{n+1} + D_{yy} \mu^{n+1}) = 0
\]

\[
\mu^{n+1} - (c^n)^3 + c^{n+1} + C^2 (D_{xx} c^{n+1} + D_{yy} c^{n+1}) = 0
\]  

\[
\begin{bmatrix}
\frac{1}{\Delta t} I + D_x u^n + D_y v^n & \frac{1}{Pe} (D_{xx} + D_{yy}) \\
I + C^2 (D_{xx} + D_{yy}) & I
\end{bmatrix}
\begin{bmatrix}
c^{n+1} \\
\mu^{n+1}
\end{bmatrix} =
\begin{bmatrix}
\frac{c^n}{\Delta t} \\
(c^n)^3
\end{bmatrix}
\]

\[
-(D_{xx} + D_{yy}) \omega = h \quad (12a)
\]

\[-(D_{xx} + D_{yy}) \psi = \omega \quad (12b)
\]

\[
u = D_x \psi \quad ; \quad v = -D_y \psi
\]  

where \( \Delta t \) is the time step, \( n \) is time level and \( I \) is identity matrix.

The implementation of the algorithm of the numerical method described above is as follows:

1. Initialize \( t = 0, n = 0, (u^n, v^n, \omega^n, \psi^n, c^n, \mu^n) \).
2. Time increment \( t^{n+1} = t^n + \Delta t \).
3. Solve Equation 12a and 12b, to obtain the vorticity and stream function\((\omega^{n+1}, \psi^{n+1})\).
4. Solve Equation 13, to obtain the flow field\((u^{n+1}, v^{n+1})\).
5. Solve Equation 11 iteratively using Picard linearization to obtain the concentration and the potential\((c^{n+1}, \mu^{n+1})\).
6. Set \([u \ v \ \omega \ \psi \ c \ \mu]^n = [u \ v \ \omega \ \psi \ c \ \mu]^{n+1}\).
7. Check if it has reached the maximum time limit or not, if not back to step 2.
8. Write the data and finish here.
Results and Discussion

In this section, the capability of the meshless RBF method for simulating the dynamic morphology of the interface are presented using two simulations. First simulation is the coalescence of two drops and the second simulation is the break-up of single drop.

1.1. Coalescence of two-drops

The simulation is performed on a rectangular domain with the dimensions (-1,-1) in the left bottom corner and (1,1) in the top right corner. The number of nodes is 71×71 which are distributed uniformly in the domain. The initial conditions for the shear flow are \( \psi(x,y) = 0.5y^2, \omega(x,y) = 1 \), \( u(x,y) = y, v(x,y) = 0 \) (see Figure 1) and for the concentration is expressed as follows:

\[
\begin{align*}
  c(x,y) &= \tanh\left((0.2625 - (x - 0.1825)^2 + (y - 0.240)^2)^{0.5}/2\sqrt{2} \cdot c\right) + \\
  \tanh\left((0.2625 - (x + 0.1825)^2 + (y + 0.240)^2)^{0.5}/2\sqrt{2} \cdot c\right) + 1.0
\end{align*}
\] (14)

The boundary conditions for the flow field are Dirichlet boundary conditions, by prescribed the value using the initial conditions at the boundaries. The boundary conditions of the potential and the concentration are constant, i.e., \( \mu = 0 \) and \( c = -1 \) due to the interface never reach the boundaries.

![Figure 1](image1.png)  
**Figure 1** Domain geometry, nodes distribution and velocity field for the simulation of coalescence of two drops

Figure 2 shows the evolution of the coalescence the two-drops for the value \( C = 0.02, \ Pe = 50, Ca = 0.1 \) and \( \Delta t = 0.0005 \). Initially two identical drops are placed on the middle of the domain as shown in Figure 2(a). Then the droplet will approach each other while experiencing stretched by shear flow (see Figure 2(b)). After the two droplets touch, the two droplets merge first to form like a dumbbell as shown in Figure 2(c), then the touched area increases as shown in Figure 2(d), so that the combined shape will be angled ellipsoidal. This slope is affected by the presence of a shear flow that pulls the top droplet to the right and the bottom droplet to the left.
Figure 2 Evolution of coalescence of two drops in a linear shear flow: (a) $t = 0.0$, (b) $t = 0.1$, (c) $t = 0.2$, and (d) $t = 0.3$

1.2. Break-up of single drop

Similar to the first simulation, the second simulation is performed on a rectangular domain with the dimensions (-1,-0.5) in the left bottom corner and (1, 0.5) in the top right corner. The number of nodes is 71×36 which are distributed uniformly in the domain. The initial conditions for the shear flow are $\psi(x, y) = 4y^2$, $\omega(x, y) = 8$, $u(x, y) = 8y$, $v(x, y) = 0$ and for the concentration is expressed as follows:

$$c(x, y) = \tanh\left(\frac{0.25 - ((x - 0)^2 + (y - 0)^2)^{0.5}}{2\sqrt{2}C}\right)$$

(15)

The boundary conditions for the flow field are Dirichlet boundary conditions, the same as described in the first simulation. Figure 3 shows the domain and the node distribution.

Figure 3 Domain geometry, nodes distribution and velocity field for the simulation of break-up of single drop

Figure 4 shows the evolution of the coalescence the two-drops for the value $C = 0.04$, $Pe = 2.5$, $Ca = 10$ and $\Delta t = 0.0005$. The initial shape of the drop is circular then stretched by the shear flow and becomes ellipsoidal (see the evolution from Figure 4(a) and so on). The mayor axis lengthens and the minor axis shrinks, and the center of the droplet becomes thinner. At the end the droplet breaks-up into two smaller droplets, as shown in Figure 4(j).
Figure 4 Evolution of break-up of single drop in a linear shear flow: (a) $t = 0.0$, (b) $t = 0.1$, (c) $t = 0.2$, (d) $t = 0.3$, (e) $t = 0.4$, (f) $t = 0.5$, (g) $t = 0.6$, (h) $t = 0.7$ (i) $t = 0.8$, and (j) $t = 0.9$
Conclusion
We have proposed meshless radial basis function method combined with the Cahn-Hilliard equation to simulate the two phase flow model in low velocity flow field. The proposed method is then employed for simulating the coalescence and break up drops in steady shear flow. The simulations show that the dynamic of complex morphology of the interface can be captured easily. In our next research plan, we want to investigate the effect of density ratio, viscosity ratio, thermal, and Reynolds number.

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