 FDMP, vol.7, no.3, pp.231-240, 2011

Numerical Simulation of an Axisymmetric Compound Droplet by Three-Fluid Front-Tracking Method

S. Homma[1], M. Yokotsuka[1], T. Tanaka[1], K. Moriguchi[1], J. Koga[1] and G. Tryggvason[2]

Abstract: We develop a three-fluid front-tracking method in order to simulate the motion of an axisymmetry compound droplet, which consists of three immiscible fluids separated by two different interfaces. The two interfaces of the compound droplet are represented by two different sets of the front-tracking elements immersed on the Eulerian grid mesh, where the velocities and the pressure are calculated. The density and viscosity profiles with jumps at the interfaces are successfully determined from the location and the connection information of the front-tracking elements. The motion of a compound droplet is simulated on axisymmetric cylindrical coordinates. The results show that the three-fluid front tracking method works appropriately for the motion of a compound droplet. Stability of a spherical compound droplet is examined numerically and the stable position is found from the simulations.

Keywords: three immiscible fluids, interface, front-tracking method, compound droplets.

1 Introduction

Although the flow involving three distinct fluids is rather complex, it is often encountered in industrial processes. Double emulsion is one example (Gart, 1997). This is highly structured fluids of emulsion drops that contain smaller droplets inside. The emulsion drop of this type is usually referred as a compound droplet, which consists of two immiscible phases in yet another immiscible continuous phase. The fluid dynamics of the compound droplets has been studied (Johnson and Sadhal, 1985), and it has still attracted considerable attention, partly because of its potential to manufacture highly structural materials such as micro capsules for drug delivery vehicle (Prankerd and Stella, 1990).

[1] Saitama University, Saitama, Japan
[2] University of Notre Dame, Notre Dame, IN, U.S.A.

In this study, we develop a three-fluid front-tracking method based on the original front-tracking method (Unverdi and Tryggvason, 1992) in order to simulate the motion of an axisymmetric compound droplet that consists of three immiscible fluids separated by two different interfaces. The two interfaces of the compound droplet are represented by two different sets of the front-tracking elements immersed on the Eulerian grid mesh, where the velocities and the pressure are calculated.

This paper is organized as follows: After describing how the front-tracking method is modified, the density and viscosity profiles are shown to verify if the modified front-tracking method successfully determines the densities and viscosities with jumps at the interfaces. The motion of a compound droplet is discussed by comparing with the theoretical and numerical results for a spherical compound droplet in a uniform flow (Sadhal and Oguz, 1985).

2 Governing equations and numerical method

Figure 1 shows a schematic of the problem. An initially spherical compound droplet of radius R_2 is placed in a quiescent external fluid of viscosity μ_1 and density ρ_1. The compound droplet consists of a shell (μ_2 and ρ_2) and a core (μ_3 and ρ_3) whose radius is R_3. Under constant gravity, the entire droplet and the core move depending on the density difference between the external fluid and the droplet, or on that between the shell and core fluids. The droplet eventually reaches the terminal velocity balancing the buoyancy force with the viscous drag force. The entire droplet and the core can be deformed depending on the relative contribution of the interfacial tension to the other forces.

If the external fluid and the compound droplet are assumed to be incompressible and Newtonian, the governing equations for one-fluid formulation (Unverdi &Tryggvason, 1992) are the continuity equation, the Navier-Stokes equation, and the equations of state for density and viscosity:

$$\nabla \cdot \mathbf{u} = 0, \tag{1}$$

$$\frac{\partial}{\partial t}\rho\mathbf{u} + \nabla \cdot \rho\mathbf{u}\mathbf{u} = -\nabla P + \nabla \cdot \mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T) + \rho\mathbf{g} + \int_f \sigma\kappa\mathbf{n}_f\delta(\mathbf{x}-\mathbf{x}_f)dA_f, \tag{2}$$

$$\frac{D}{Dt}\rho = \frac{D}{Dt}\mu = 0. \tag{3}$$

Here, $\mathbf{u}$ is the velocity vector, P the pressure, ρ the density, μ the viscosity, σ the interfacial tension coefficient, and$t$ the time. The interfacial tension is found using twice the mean curvature, κ, the unit normal, $\mathbf{n}_f$, and a delta function, $\delta(\mathbf{x}-\mathbf{x}_f)$, which is zero everywhere except at the interface, $\mathbf{x}_f$.

Equations (1) and (2) are discretized on the axisymmetric cylindrical coordinate by finite difference approximations with second order. The boundary conditions of the left-side of the domain (z-axis) are symmetry, and the other boundaries are no-slip-wall. The initial velocities are zero ($\mathbf{u}_0 \equiv 0$) as the fluid is at rest. The motion of the interface is traced by a front-tracking method (Unverdi and Tryggvason, 1992). The details of the front-tracking method were described by Tryggvason *et al.* (2001), and the axisymmetric version of the front-tracking method was examined in jet breakup problems by Homma *et al.* (2006).

For the front-tracking method by Tryggvason *et al.* (2001), the density and viscosity fields are determined by an indicator function, defined, for example, by $I = 1$ for fluid 1 and $I = 0$ for fluid 2. Since the indicator function depends on the location of interfaces, it is necessary to determine the function every time step from the locations of the front elements. The gradient of I has a value only at the interface and can be expressed as

$$\nabla I = \int_f \Delta I \mathbf{n}_f \delta(\mathbf{x} - \mathbf{x}_f) dA_f. \tag{4}$$

Taking divergence of Eq. (4) results in the Poisson equation

$$\nabla^2 I = \nabla \cdot \int_f \Delta I \mathbf{n}_f \delta(\mathbf{x} - \mathbf{x}_f) dA_f \,. \tag{5}$$

The right hand side can be calculated from the information of the front elements and ΔI is unity for the above example. The left-hand side is approximated by standard centered differences, and solving the Poisson equation with the appropriate boundary conditions yields the field of the indicator function everywhere.

For three-fluid front tracking method, we use an indicator function defined by

$$I(\mathbf{x},t) = \begin{cases} 1 & \text{a fluid with maximum density (MXD)} \\ 0 & \text{a fluid with intermediate density (IMD)} \\ -1 & \text{a fluid with minimum density (MND)} \end{cases} \tag{6}$$

In this case, ΔI is 1 for the interface between MXD and IMD and is -1 for that between IMD and MND. Once the indicator function is determined, we can calculate the density from

$$\begin{aligned} \rho(\mathbf{x},t) = & \max(\rho_1,\rho_2,\rho_3) \cdot \max(I(\mathbf{x},t),0) \\ & + [(\rho_1+\rho_2+\rho_3) - \max(\rho_1,\rho_2,\rho_3) - \min(\rho_1,\rho_2,\rho_3)] \\ & \cdot (1 - sgn(I(\mathbf{x},t)) \cdot I(\mathbf{x},t)) \\ & - \min(\rho_1,\rho_2,\rho_3) \cdot \min(I(\mathbf{x},t),0) \,. \end{aligned} \tag{7}$$

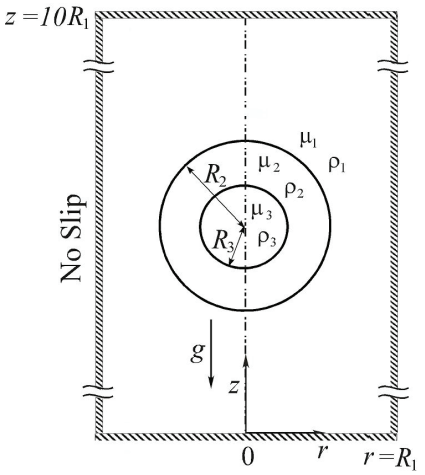

Figure 1: Computational domain for simulation of a compound droplet.

The viscosity can be determined by a similar manner to the density.

3 Results and discussion

3.1 Density and viscosity field

In order to check whether the density and viscosity are obtained correctly, those distributions are plotted for a spherical compound droplet ($R_2 = 0.3$ and $R_3 = 0.2$) as shown in **Fig. 2**. The ratios of density and viscosity in this case are as follows: $\rho_2/\rho_1 = 2$, $\rho_3/\rho_1 = 0.5$, $\mu_2/\mu_1 = 2$ and $\mu_3/\mu_1 = 3$. The cross-sectional distributions along the center (a broken line in the top figures) of the compound droplet show that the density and viscosity with jumps at the interfaces are successfully determined (bottom figures). Thus, the algorithm based on Eqs. (5)-(7) works appropriately in the three-fluid front tracking method.

3.2 Motion of a spherical compound droplet

Sadhal and Oguz (1985) studied theoretically the translatory motion of a compound droplet for low-Reynolds-number flow. The solution is limited to small capillary number ranges, where the interfacial tension overcomes the viscous forces, thereby keeping the compound droplet spherical during the translation. One important result of their study is stability of the position of the core droplet inside the shell droplet. The stable position depends on the density ratios between core and shell droplets. **Figure 3** shows the relative translation velocity of the core droplet to the

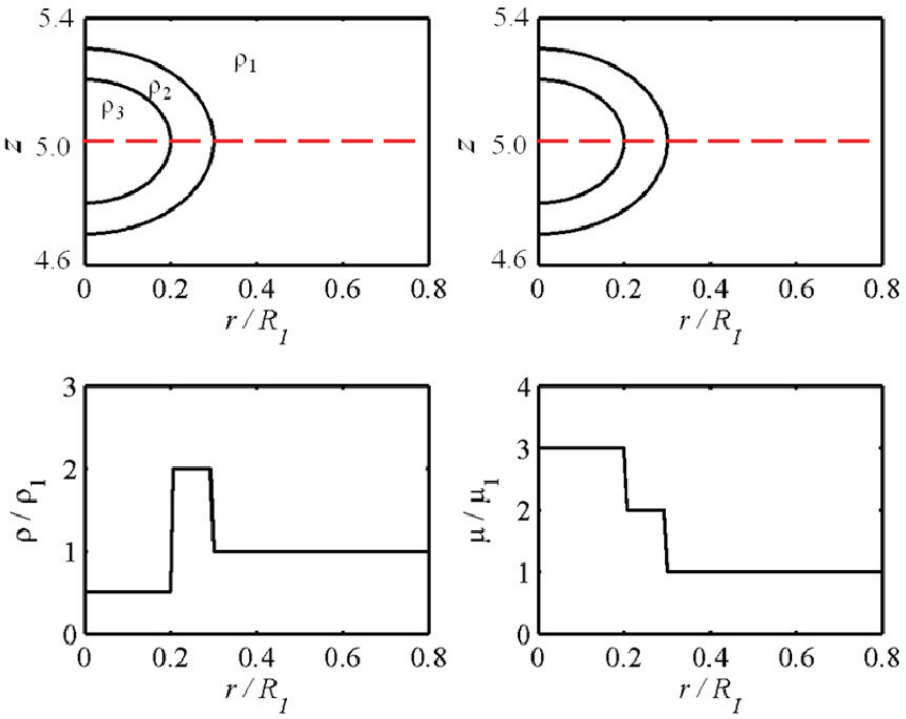

Figure 2: Density (left) and viscosity (right) distributions determined from the position of the front-tracking elements.

shell droplet (V) as a function of eccentricity, which is the position relative to the compound droplet itself (shell droplet). The eccentricity is defined by $\varepsilon = d/(R_2 - R_3)$, see **Fig. 4**. The intersections between the curves and the line $V/U = 0$, where U is the translation velocity of the compound droplet itself or the velocity of the external flow, show the equilibrium points. There are three kinds of equilibrium points: stable, unstable, and metastable ($\varepsilon = 0$). In this study, whether the stable equilibrium is attainable, is tested by our numerical simulations. Since the aim of this section is to compare our numerical results with the theoretical ones, the condition similar to their study has been used in our simulations; the order of the capillary number ($\mathrm{Ca} = \mu U/\sigma$), for example, is 10^{-2}.

Figure 5 shows three eccentric configurations for $R_2/R_3 = 0.5$ and $\mu_2/\mu_1 = \mu_3/\mu_1 = 1$. The density ratio between external fluid and shell droplet (ρ_2/ρ_1) is fixed at 1.2, resulting in the downward buoyancy force acting on the compound droplet itself. The configuration depends on the density ratio between external fluid and

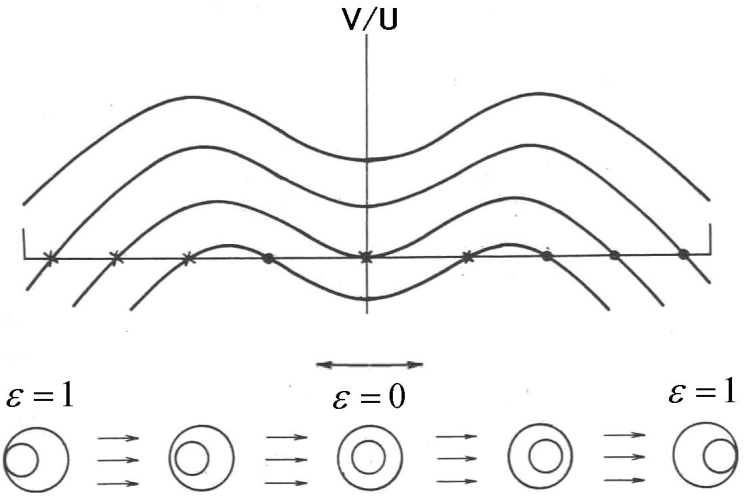

Figure 3: Schematic of the core droplet velocity as a function of its relative position (Sadhal and Oguz, 1985): • stable equilibrium, ×unstable equilibrium.

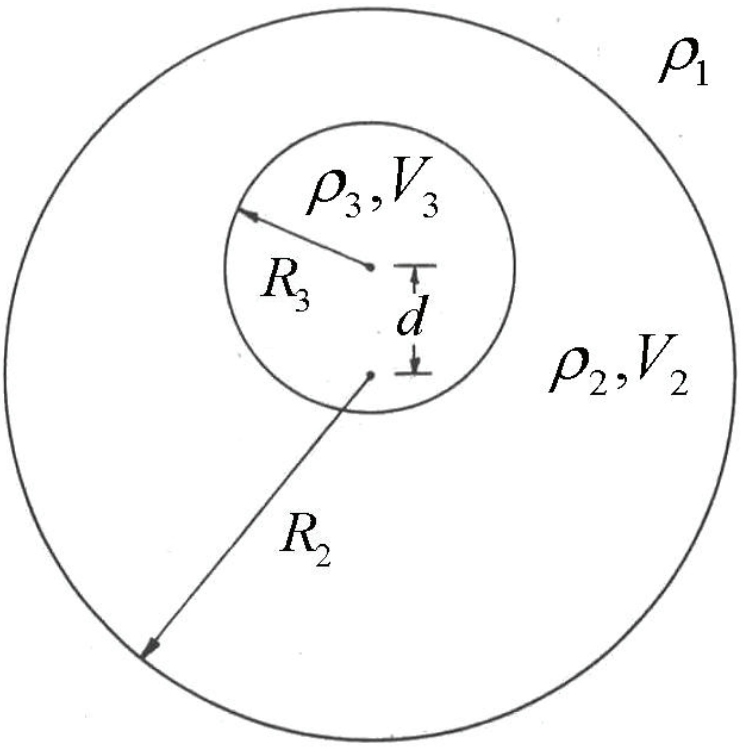

Figure 4: Schematic of the definition of eccentricity.

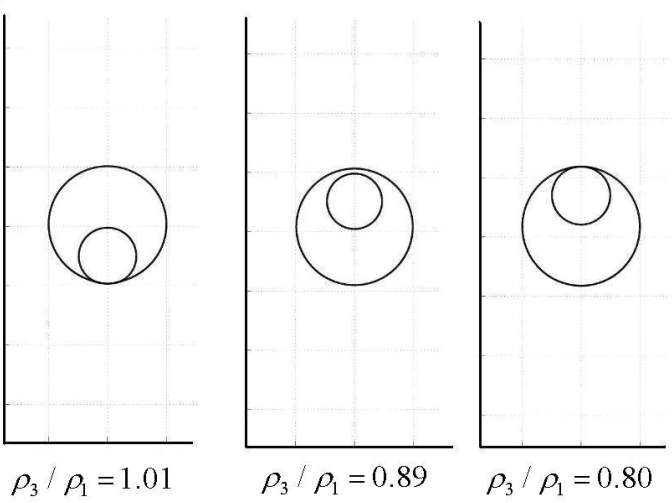

Figure 5: Eccentric configurations for $\mu_2/\mu_1=\mu_3/\mu_1=1$ and $\rho_2/\rho_1 = 1.2$.

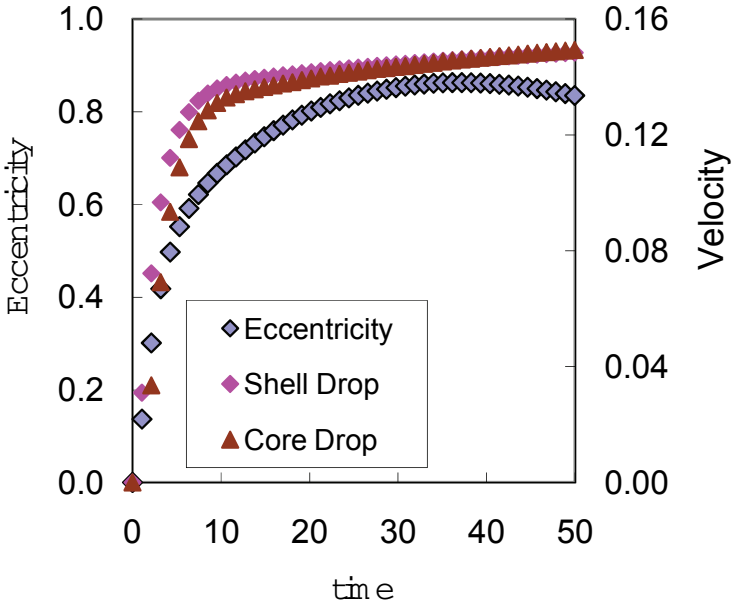

Figure 6: Eccentricity and velocities for stable equilibrium configuration ($\rho_3/\rho_1 = 0.89$).

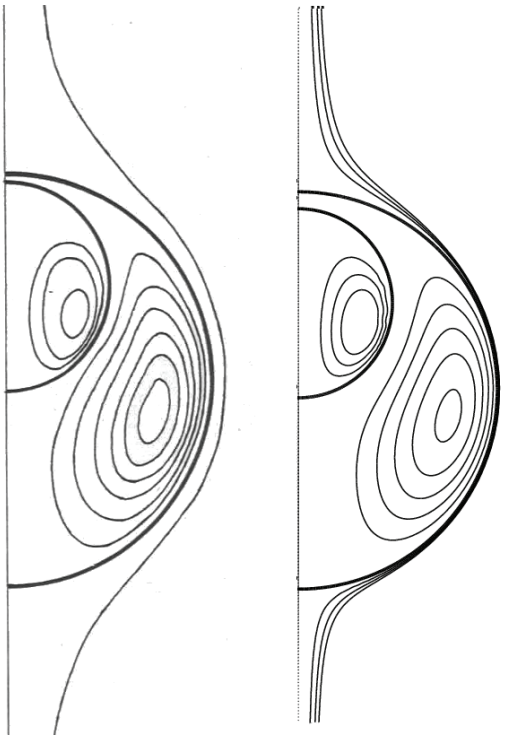

Figure 7: Comparison of the flow stream lines between exact solution (left: $\varepsilon = 0.9$, Sadhal and Oguz, 1985) and front-tracking simulation (right: $\varepsilon = 0.89$)

core droplet (ρ_3/ρ_1). In the case of $\rho_3/\rho_1 = 1.01$, the core droplet falls with shell droplet because the average density of the compound droplet is larger than the external fluid. In this case, $\varepsilon = 1$ and it is unstable equilibrium (the most left point in Fig. 3). For $\rho_3/\rho_1 = 0.89$, the core droplet does not touch the top of the shell droplet and the entire droplet falls holding this configuration. This case shows the stable equilibrium, where buoyancy force balances with viscous forces. The flow pattern and the dynamics of eccentricity in this case will be shown later. In the case of $\rho_3/\rho_1 = 0.8$, a similar eccentric configuration to $\rho_3/\rho_1 = 0.89$ is observed, but the core droplet touches the top interface of the shell droplet. This is also stable equilibrium configuration (the most right point in Fig. 3).

Note that nothing wrong happens when two different interfaces touch as in the case of $\rho_3/\rho_1 = 1.01$ and 0.80. Even when two different interfaces touch and the both front elements are positioned in one grid mesh, where pressure and velocities are calculated, the indicator function is appropriately determined by solving Eq. (5)

and the value will be an average depending on the location of the front elements. The densities and viscosities around the grid mesh are also determined appropriately by the appropriate values of the indicator function. Furthermore, the pressures around the grid mesh are appropriately determined incorporating the interfacial tensions by the two different interfaces. The situation where two different interfaces touch often occurs even in two-fluid cases and the front-tracking method properly handles this situation.

Figure 6 shows the dynamics of eccentricity and the velocities of core and shell droplets for $\rho_3/\rho_1 = 0.89$. The velocity of the shell droplet increases slightly faster than that of the core droplet, and those velocities eventually equalize. Thus, V/U becomes 0 and the compound droplet attains an equilibrium configuration. The eccentricity increases and reaches around 0.8.

Figure 7 shows the comparison of the flow stream lines inside and around the compound droplet between exact solution (Sadhal and Oguz, 1985) and front-tracking simulation. The eccentricities of the exact solution and the front-tracking simulation are 0.9 and 0.89, respectively. There are double vortices inside the compound droplet. The stream lines are slightly different in the exterior of the droplet. This seems to be caused by the difference of the computational method. Sadhal and Oguz obtained the steady state solutions under constant velocity of the external fluid (U). We, on the other hand, solved unsteady Navier-Stokes equations and the translation velocity of the droplet (U) was the solution. Although the stream lines in the external fluid are slightly different, the flow patterns of both the exact solution and the front-tracking simulation are almost the same. The three-fluid front-tracking method developed in this study, therefore, can reasonably simulate the translation of a spherical compound droplet.

4 Conclusions

Three-fluid front-tracking method is developed in order to simulate the motion of an axisymmetric compound droplet that consists of three immiscible fluids separated by two different interfaces. The two interfaces of the compound droplet are represented by two different sets of the front-tracking elements immersed on the Eulerian grid mesh, where the velocities and the pressure are calculated. The density and viscosity profiles with jumps at the interfaces are successfully determined from the location and the connection information of the front-tracking elements. The translatory motion of a compound droplet is simulated on axisymmetric cylindrical coordinates. The results show that the three-fluid front tracking method works appropriately for the translation of a compound droplet. Stability of a spherical compound droplet is examined numerically and the stable position is found from the simulations. This is in good agreement with theoretical study by Sadhal

and Oguz (1985).

References

Gart, N. (1997): Double emulsions - scope, limitations and new achievements. *Colloids and Surfaces A*: *Physicochemical and Engineering Aspects* 123-124, pp. 233-246.

Homma, S.; Koga, J.; Matsumoto, S.; Song, M.; Tryggvason, G. (2006): Breakup mode of an axisymmetric liquid jet injected into another immiscible liquid. *Chemical Engineering Science*, vol. 61, pp. 3986-3996.

Johnson, R. E.; Sadhal, S. S. (1985): Fluid mechanics of compound multiphase drops and bubbles. *Annual Review of Fluid Mechanics*, vol. 17, pp. 289-320.

Prankerd, R. J.; Stella, V. J. (1990): The use of oil-in-water emulsions as a vehicle for parenteral drug administration. *Journal of Parenteral Science and Technology*, vol. 44, No. 3, pp. 139-149.

Sadhal, S.; Oguz, H. N. (1985): Stokes flow past compound multiphase drops: the case of completely engulfed drops/bubbkes. *Journal of Fluid Mechanics*, vol. 160, pp. 511-529.

Tryggvason, G.; Bunner, B.; Esmaeeli, A.; Juric, D.; Al-Rawahi, N.; Tauber, W.; Han, J.; Nas, S.; Jan, Y. (2001): A front-tracking method for the computations of multiphase flow. *Journal of Computational Physics*, vol. 169, pp. 708-759.

Unverdi, S. O.; Tryggvason, G. (1992): A front-tracking method for viscous, incompressible, multi-fluid flows. *Journal of Computational Physics*, vol. 100, pp. 25-37.