Chapter 7

Ternary Navier-Stokes-Cahn-Hilliard system

Many engineering and industrially important applications involve flows with more than two liquid components. Therefore, I developed an extension of the diffuse interface model and numerical algorithms to the case of ternary (three-phase) fluid flows. In the Boussinesq limit, the ternary Navier-Stokes-Cahn-Hilliard system is

$$\begin{aligned}
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} &= -\nabla p + \nabla\cdot\left[\eta\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right)\right] - \sigma_i\epsilon(\Delta c_i \nabla c_i - \frac{1}{2}\nabla|\nabla c_i|^2) && (7.0.1)\\
&\quad + \rho g\mathbf{G}, && (7.0.2)\\
\nabla\cdot\mathbf{u} &= 0, && (7.0.3)\\
\frac{\partial c_1}{\partial t} + \nabla\cdot(c_1\mathbf{u}) &= \nabla\cdot(M_1(c_1,c_2)\nabla\mu_1), && (7.0.4)\\
\frac{\partial c_2}{\partial t} + \nabla\cdot(c_2\mathbf{u}) &= \nabla\cdot(M_2(c_1,c_2)\nabla\mu_2), && (7.0.5)
\end{aligned}$$

where the c_1, c_2, and $c_3 = 1 - c_1 - c_2$ are the mass ratios of the components, σ_i satisfies the relation, $\sigma_{ij} = \sigma_i + \sigma_j$, where σ_{ij} is the surface tension between i component and j component. ρ is density, ϵ is a measure of interface thickness, and the chemical potentials are given by

$$\begin{aligned}
\mu_1 &= \frac{\partial F}{\partial c_1}(c_1,c_2) - 2\epsilon^2\Delta c_1 - \epsilon^2\Delta c_2, && (7.0.6)\\
\mu_2 &= \frac{\partial F}{\partial c_2}(c_1,c_2) - \epsilon^2\Delta c_1 - 2\epsilon^2\Delta c_2, && (7.0.7)
\end{aligned}$$

where $F(c_1, c_2)$ is Helmholtz free energy.

7.1 Hydrodynamics of a compound drop with application to leukocyte modeling

Leukocytes (white blood cells) play a key role in the human immune defense network. In the course of carrying out their functions, they must undergo large deformations as they navigate through small apertures in the tissues. The ability of leukocytes to deform and flow in capillaries and to migrate in tissues is largely governed by their rheological properties. Therefore, knowledge of the rheological properties of leukocytes is critical not only for the comprehension of microcirculatory system, but also for the understanding of their functions and behavior in health and disease [73]. In this chapter, we study the dynamics of a compound liquid drop which is comprised of an outer membrane surface, a shell layer, and a core. The deformation due to an imposed shear boundary flow and the subsequent recovery are investigated computationally employing a diffuse-interface method. The numerical method allows for large viscosity and capillarity differences between layers.

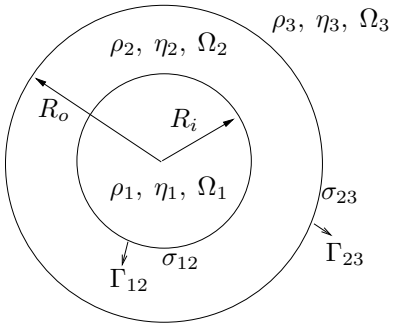


Figure 7.1: Illustration of the parameters in the analysis.

1.A Governing equations

The deformation and recovery of a viscous drop subjected to different flow conditions is investigated by a three-layer incompressible Newtonian fluid system of density ρ_i and viscosity η_i, which occupies the regions Ω_i $(i = 1, 2, 3)$, will be adopted to define the problems under investigation. In the case of a compound drop, $\Omega_1,\ \Omega_2,$ and Ω_3 represent core (or nucleus), shell (or cytoplasm), and the suspending fluid, respectively. The suface tensions σ_{12} and σ_{23} at the two interfaces Γ_{12} and Γ_{23}, are assumed to be constant. The lengths R_o and R_i are the undeformed radii of the drop (or cell) and core (or nucleus),

repectively. The choices of characteristic velocity, length, time, and pressure are as follows:

$$l_c = R_o,\ \ u_c = \frac{\sigma_{23}}{\eta_3},\ \ t_c = \frac{R_o\eta_3}{\sigma_{23}},\ \ p_c = \frac{\eta_3 u_c}{l_c},$$

where u_c is the charateristic velocity scale. Here, we consider density matched case. Based on the reference scales, the dimensionless governing equations for Navier-Stokes flows are:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla p + \frac{1}{\mathbf{Re}}\nabla\cdot\left[\eta(\nabla\mathbf{u} + \nabla\mathbf{u}^T)\right] - \frac{\epsilon}{\mathbf{We}_i}(\Delta c_i \nabla c_i - \frac{1}{2}\nabla|\nabla c_i|^2)$$

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

$$\frac{\partial c_1}{\partial t} + \nabla\cdot(c_1\mathbf{u}) = \frac{1}{\mathbf{Pe}_1}\Delta\mu_1, \tag{7.1.8}$$

$$\frac{\partial c_2}{\partial t} + \nabla\cdot(c_2\mathbf{u}) = \frac{1}{\mathbf{Pe}_2}\Delta\mu_2, \tag{7.1.9}$$

$$\mu_1 = \frac{\partial F(c_1,c_2)}{\partial c_1} - 2\epsilon^2\Delta c_1 - \epsilon^2\Delta c_2, \tag{7.1.10}$$

$$\mu_2 = \frac{\partial F(c_1,c_2)}{\partial c_2} - \epsilon^2\Delta c_1 - 2\epsilon^2\Delta c_2, \tag{7.1.11}$$

$$F(c_1,c_2) = \frac{1}{4}(c_1^2c_2^2 + c_2^2c_3^2 + c_3^2c_1^2) = \frac{1}{4}[c_1^2c_2^2 + (c_1^2+c_2^2)(1-c_1-c_2)^2]. \tag{7.1.12}$$

Next, c_1 is taken to be the core mass concentration, c_2 is the shell mass concentration and c_3 is the suspending fluid mass concentration. The domain is $[0,\ 4]\times[0,\ 2]\times[0,\ 2]$. The mesh size is $64\times32\times32$ and in the simulation, periodic boundary conditions are taken for x and y and no-slip conditions are used in the z direction. The simulation parameters are

$$\eta_1 = 0.5,\ \ \eta_2 = 0.5,\ \ \eta_3 = 0.5,\ \ \ \rho_1 = \rho_2 = \rho_3 = 1.0,$$
$$\lambda_1 = \eta_1/\eta_3 = 1.0,\ \ \lambda_2 = \eta_2/\eta_3 = 1.0,\ \ \ \epsilon = 0.015,\ \ \sigma = 0.1,\ \ \dot\gamma = 1.0,$$
$$\mathbf{Pe}_1 = 0.5/\epsilon,\ \ \mathbf{Pe}_2 = 0.5/\epsilon,\ \ \ \mathbf{We}_i = \rho_1 u_c^2/\sigma_i,\ \ \ \mathbf{Re} = \rho_1 l_c u_c^2/\eta_3,\ \ \ \mathbf{Ca} = \eta_3\dot\gamma R_o/\sigma_{23}$$

1.B Deformation dynamics

The recovery of a leukocyte suspending in an immiscible, quiescent fluid is investigated. A simple shear flow is selected in the present study. Fig. 7.2 shows a typical compound drop deformation under shear flow.

1.C Recovery Dynamics and the effect of core viscosity

After the drop is deformed, the flow is turned off and the drop relaxes (i.e. $t = 2.0$ from Fig. 7.2 is taken as the initial condition). This is shown in the left columns of Figs. 7.3 and 7.4, where the $c_2 = 0.5$

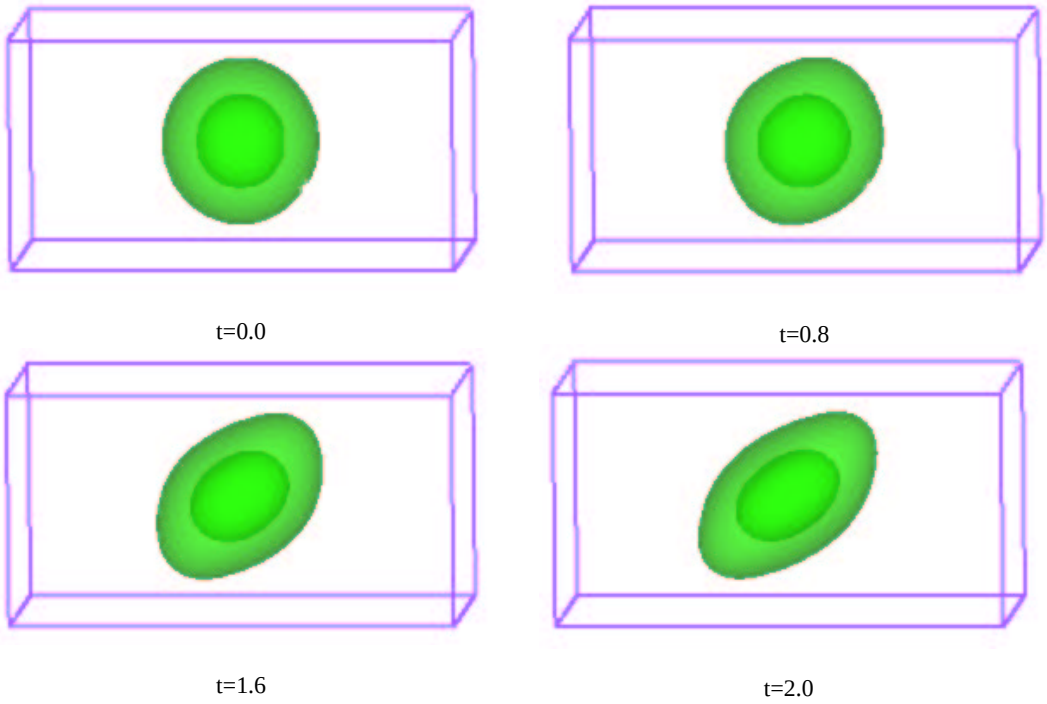


Figure 7.2: a compound drop deformation under shear flow

contours are plotted in the x-z plane with $y = 1$. The velocity vectors are also indicated. The outer interface rapidly relaxes to a sphere while the inner drop rotates and relaxes much more slowly.

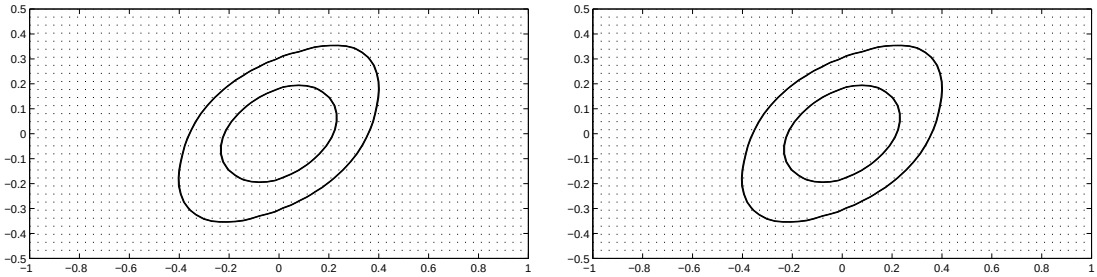
For comparision, we next consider the same initial configuration except that the viscosity of the inner drop is increased by a factor of ten to $\eta_1 = 5.0$. The results are presented in the right columns of Figs. 7.3 and 7.4. At early times, the inner interface rotates and relaxes more rapidly than the outer interface and exhibits much less deformation than the corresponding case shown in the left column. At later times, an internal velocity field is generated by the motion of the outer interface which then causes a further deformation of the inner interface.

7.2 Numerical simulation of a buoyancy-driven compound drop

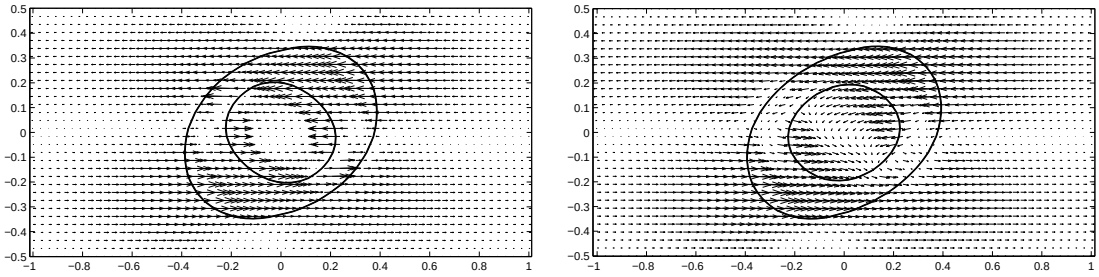
In this section, the buoyant-driven evolution a 3-D compound drop is investigated. The governing equations are:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{\mathbf{Re}} \nabla \cdot \left[\eta (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \right] - \frac{\epsilon}{\mathbf{We}_i} (\Delta c_i \nabla c_i - \frac{1}{2} \nabla |\nabla c_i|^2) + \frac{\rho - 1}{\mathbf{Fr}^2} \mathbf{G},$$

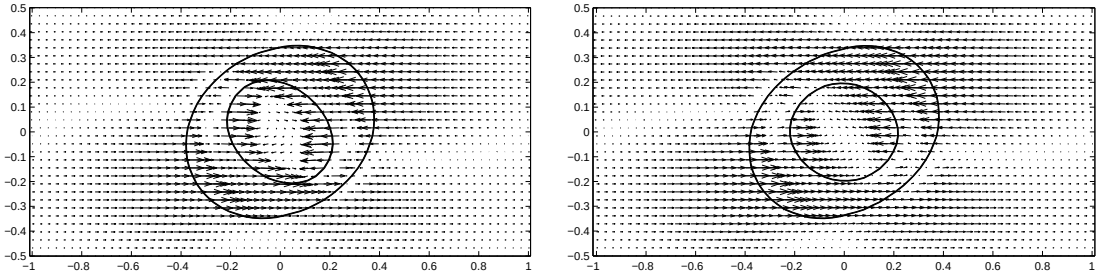
$$\nabla \cdot \mathbf{u} = 0,$$



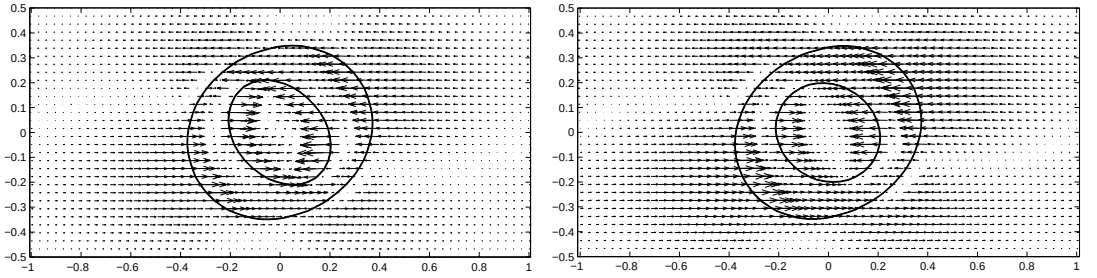
(a1) t=2.0 (b1) t=2.0



(a2) t=2.4 (b2) t=2.4

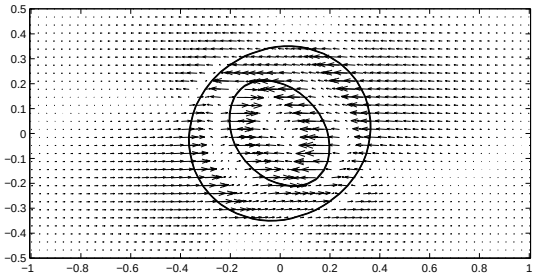


(a3) t=2.8 (b3) t=2.8

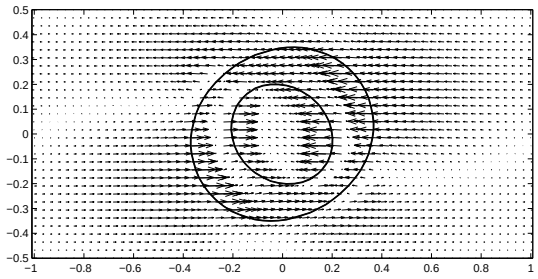


(a4) t=3.2 (b4) t=3.2

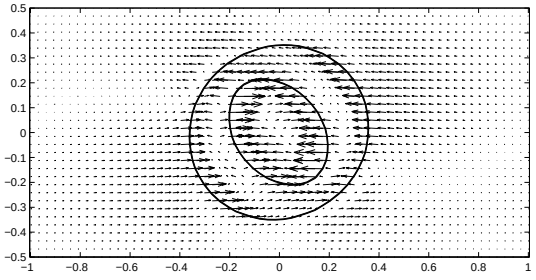
Figure 7.3: Early time: dependence of the recovery field on the viscosity of the core. Initial configuration for the $\eta_1 = 0.5$ and $\eta_1 = 5.0$ deformation are shown in (a1) and (b1). The flow fields in the recovery stages are shown in (a2)-(a4) for $\eta_1 = 0.5$ and (b2)-(b4) for $\eta_1 = 5.0$.



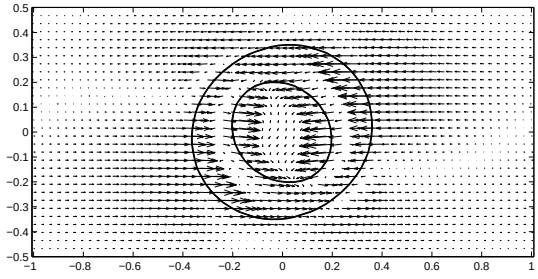
(a5) t=3.6



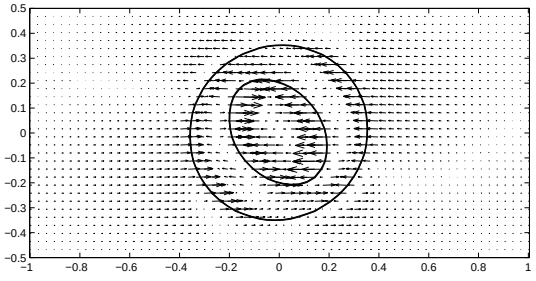
(b5) t=3.6



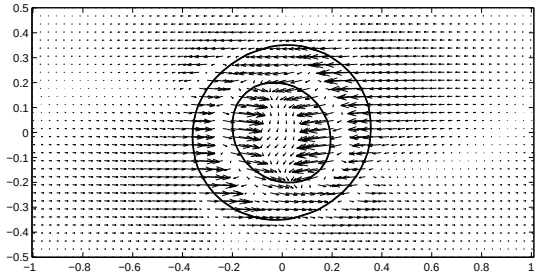
(a6) t=4.0



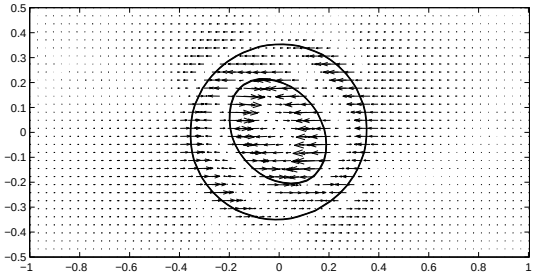
(b6) t=4.0



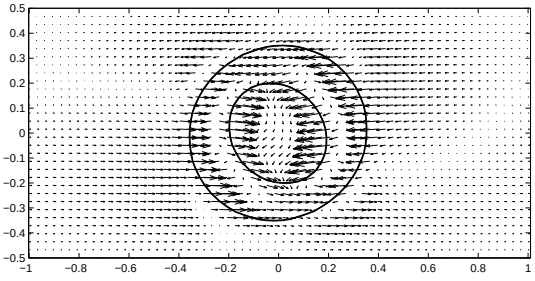
(a7) t=4.4



(b6) t=4.4



(a8) t=4.8



(b8) t=4.8

Figure 7.4: Late time continuation of Fig. 7.3 The flow fields in the recovery stages are shown in (a5)-(a8) for $\eta_1 = 0.5$ and (b5)-(b8) for $\eta_1 = 5.0$.

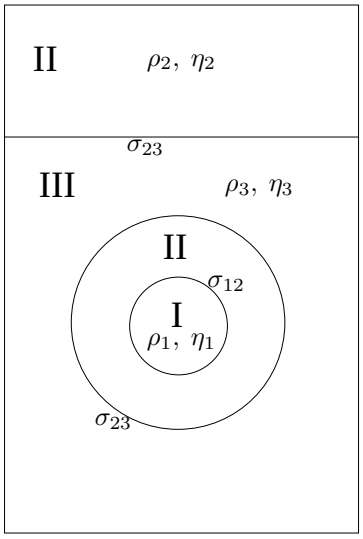


Figure 7.5: Illustration of the parameters in the analysis.

$$\begin{aligned}
\frac{\partial c_1}{\partial t} + \nabla \cdot (c_1 \mathbf{u}) &= \frac{1}{\mathbf{Pe}_1} \Delta \mu_1, \\
\frac{\partial c_2}{\partial t} + \nabla \cdot (c_2 \mathbf{u}) &= \frac{1}{\mathbf{Pe}_2} \Delta \mu_2,
\end{aligned}$$

$$\begin{aligned}
\mu_1 &= \frac{\partial F(c_1, c_2)}{\partial c_1} - 2\epsilon^2 \Delta c_1 - \epsilon^2 \Delta c_2, \\
\mu_2 &= \frac{\partial F(c_1, c_2)}{\partial c_2} - \epsilon^2 \Delta c_1 - 2\epsilon^2 \Delta c_2, \\
F(c_1, c_2) &= \frac{1}{4}(c_1^2 c_2^2 + c_2^2 c_3^2 + c_3^2 c_1^2) = \frac{1}{4}[c_1^2 c_2^2 + (c_1^2 + c_2^2)(1 - c_1 - c_2)^2].
\end{aligned}$$

In Fig. 7.5, a schematic of the initial configuration is shown. The evolution is presented in Fig. 7.6. The following parameters were used in the simulation :

$$\eta_1 = 0.1833,\ \ \eta_2 = 0.1833,\ \ \eta_3 = 0.1833,\ \ \ \rho_1 = 1.15,\ \ \rho_2 = 1.1,\ \ \rho_3 = 1.2,$$
$$\epsilon = 0.01,\ \ \ gravity = 980.0,\ \ \ \mathbf{Pe}_1 = 10.0/\epsilon,\ \ \mathbf{Pe}_2 = 10.0/\epsilon,\ \ \mathbf{Re} = 1.0.$$

An upper (flat) interface separates the heavy ambient from same fluid that encapsulates the heavy drop. The compound drop is lighter than the heavy ambient and so it rises and deforms. The encapsulating fluid rises faster than the heavy inner drop but nevertheless the compound drop remains intact until it penetrates the upper interface. The heavy inner drop is carried upwards as the encapsulated fluid is released. The drop then falls back on the interface remaining trapped there as it is neutrally buoyant with respect to the lower heavy ambient. At this point, the drop could be removed from the system by

"sucking" it off the interface. Imagining that the heavy inner drop is a contaminant in the lower ambient, this provides a mechanism by which the ambient may be cleansed. Observe that the equilibrium drop configuration (at the final time) actually has sharp corners due to the contact of all three immiscible components. The contact angle is approximately 120 degrees since the surface tensions between all the components were taken to be the same.

7.3 Rayleigh-Taylor Instability of Ternary Fluid Flows

In this section, we exploit the fact that our NSCH system is capable of describing multicomponent fluid flows containing immiscible, miscible and partially miscible components. For immiscible components, three-phase contact angles are automatically handled though the continuum formulation (e.g. see [69]). The miscibility of the components is modeled through the properties of the free energy $F(c_1, c_2)$ and the thermodynamics of ternary flows is much more complicated than for binary case. Thus it is much more difficult to describe equilibrium configurations and to construct free energies capable of describing partially miscible systems where, for example, two components are immiscible and the third component is preferentially miscible in one of the immiscible components. Nevertheless, I have been able to construct a class of such a free energies an example of which is given below:

$$F(c_1, c_2) = 2c_1^2(1 - c_1 - c_2)^2 + (c_1 + 0.2)(c_2 - 0.2)^2 + (1.2 - c_1 - c_2)(c_2 - 0.4)^2.$$

A contour plot of the free energy $F(c_1, c_2)$ is shown in Fig. 7.7. The two minima of $F(c_1, c_2)$ are at $(0.7779, 0.2330, -0.0109)$ and $(-0.0151, 0.3651, 0.6499)$.

To demonstrate the evolution possible in ternary fluid flows, I present an example in which there is a gravity-driven (Rayleigh-Taylor) instability that enhances the transfer of a preferentially miscible contaminant from one immiscible fluid to another. The initial configuration is shown in Fig. 7.8. The top half of the domain consists of a mixture of fluid I and fluid II, and the bottom half consists of fluid III, which is immiscible with fluid I. Fluid II is preferentially miscible with fluid III. Fluid I is assumed to be the lightest and fluid II the heaviest. The density of the I/II mixture is heavier than that of fluid III, so the density gradient induces Rayleigh-Taylor Instability. The simulation parameters are

$$\begin{aligned}
&\eta_1 = \eta_2 = \eta_3 = 0.1, \quad \rho_1 = 1.0, \ \ \rho_2 = 1.5, \ \ \rho_3 = 1.2, \\
&\epsilon = 0.01, \quad \text{gravity} = 980.0, \quad \mathbf{Pe}_1 = 0.5/\epsilon, \ \ \mathbf{Pe}_2 = 0.5/\epsilon, \ \ \mathbf{Re} = 10.0 \\
&\rho_1 = \frac{\sigma}{2}, \ \ \rho_2 = -\frac{\sigma}{2}, \ \rho_3 = \frac{\sigma}{2}, \ \ \sigma = 0.001.
\end{aligned}$$

As the simulation begins, in Fig. 7.9, the I/II mixture falls and fluid II diffuses into fluid III. The overall diffusion is much more rapid due to the large velocities generated in the flow that act to increase

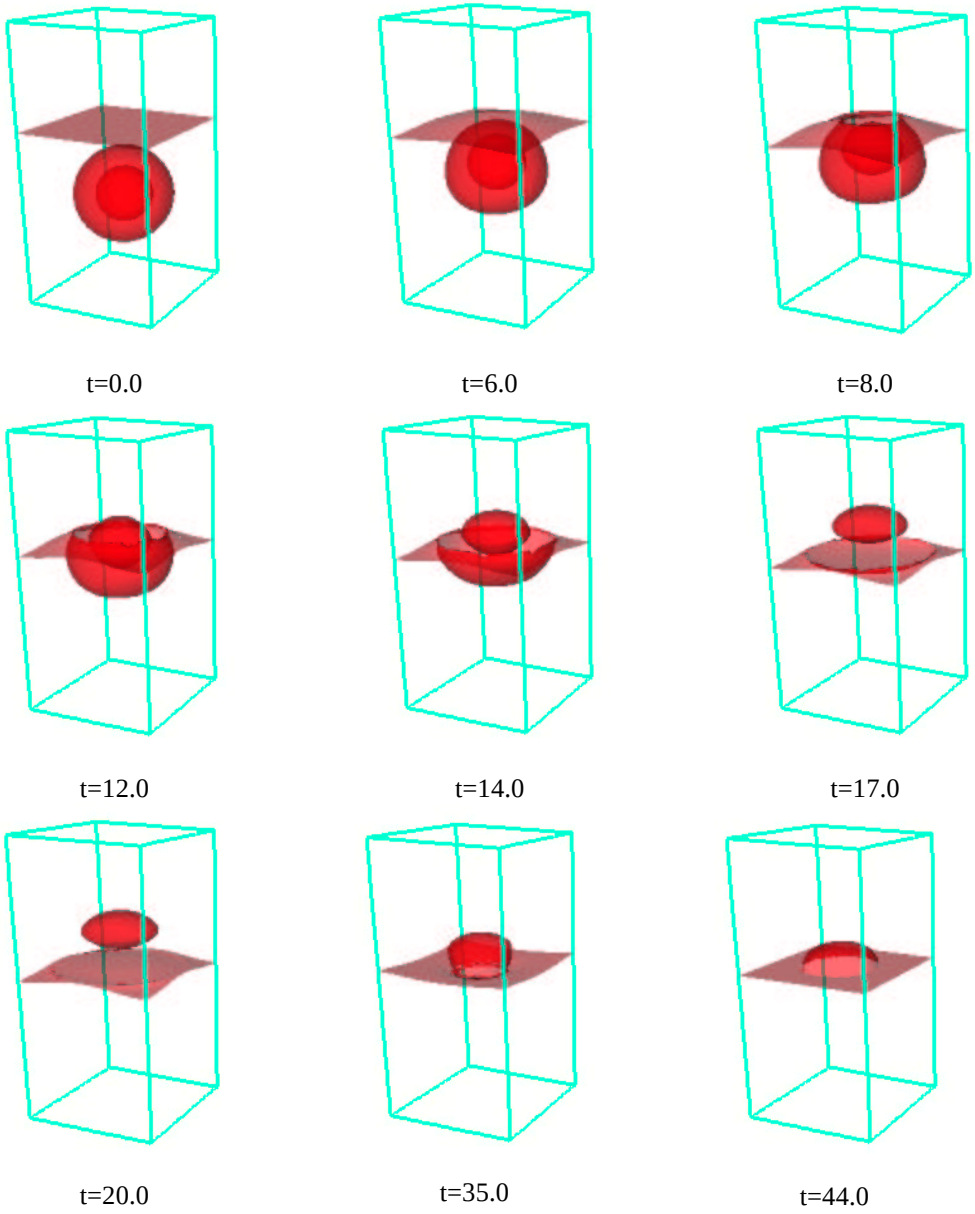


Figure 7.6: Evolution of a compound drop

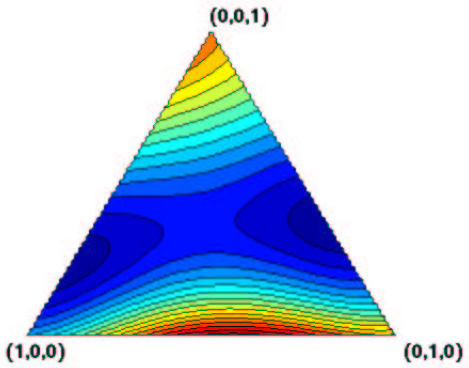


Figure 7.7: Contour plot of the free energy $F(c_1, c_2)$ on the Gibbs triangle.

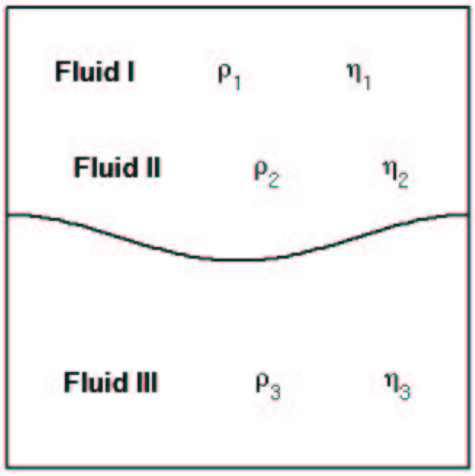
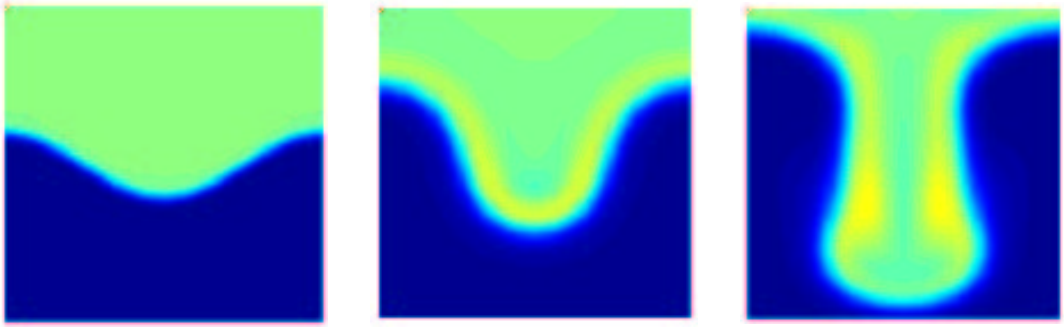
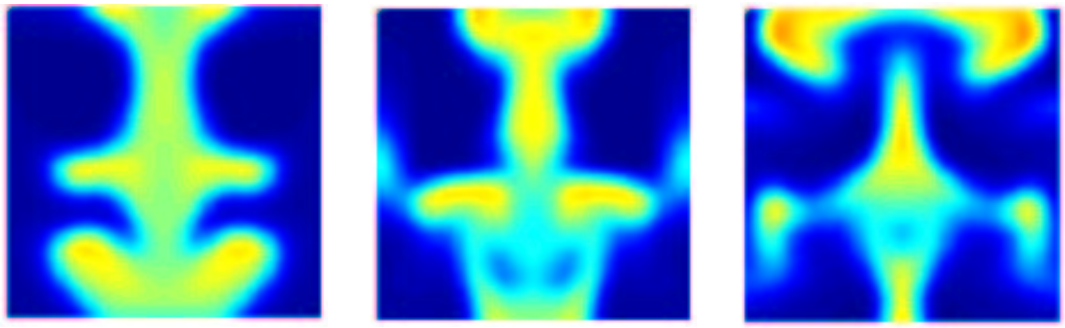


Figure 7.8: schematic of initial configuration

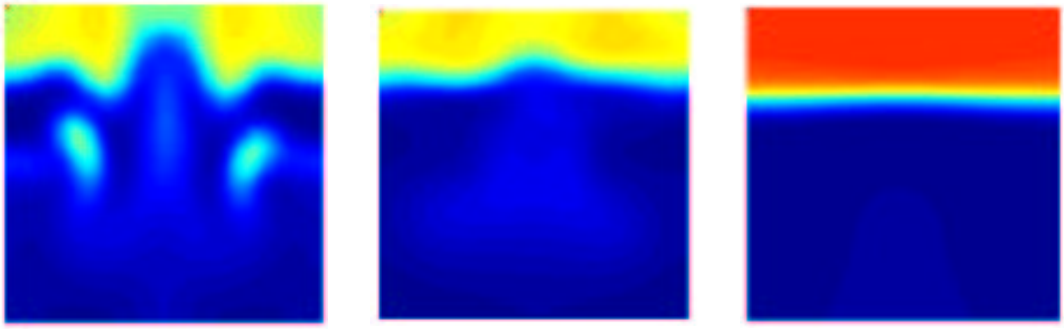
the surface area of the I/III interface. As fluid II is diffused from fluid I, the pure fluid I rises to the top as shown in Fig. 7.9. Imagining that fluid II is a contaminant in fluid I, this configuration provides an efficient means of cleansing fluid I.



t=0 t=1 t=2



t=3 t=4 t=5



t=6 t=7 t=50

Figure 7.9: Evolution of concentration of fluid I.

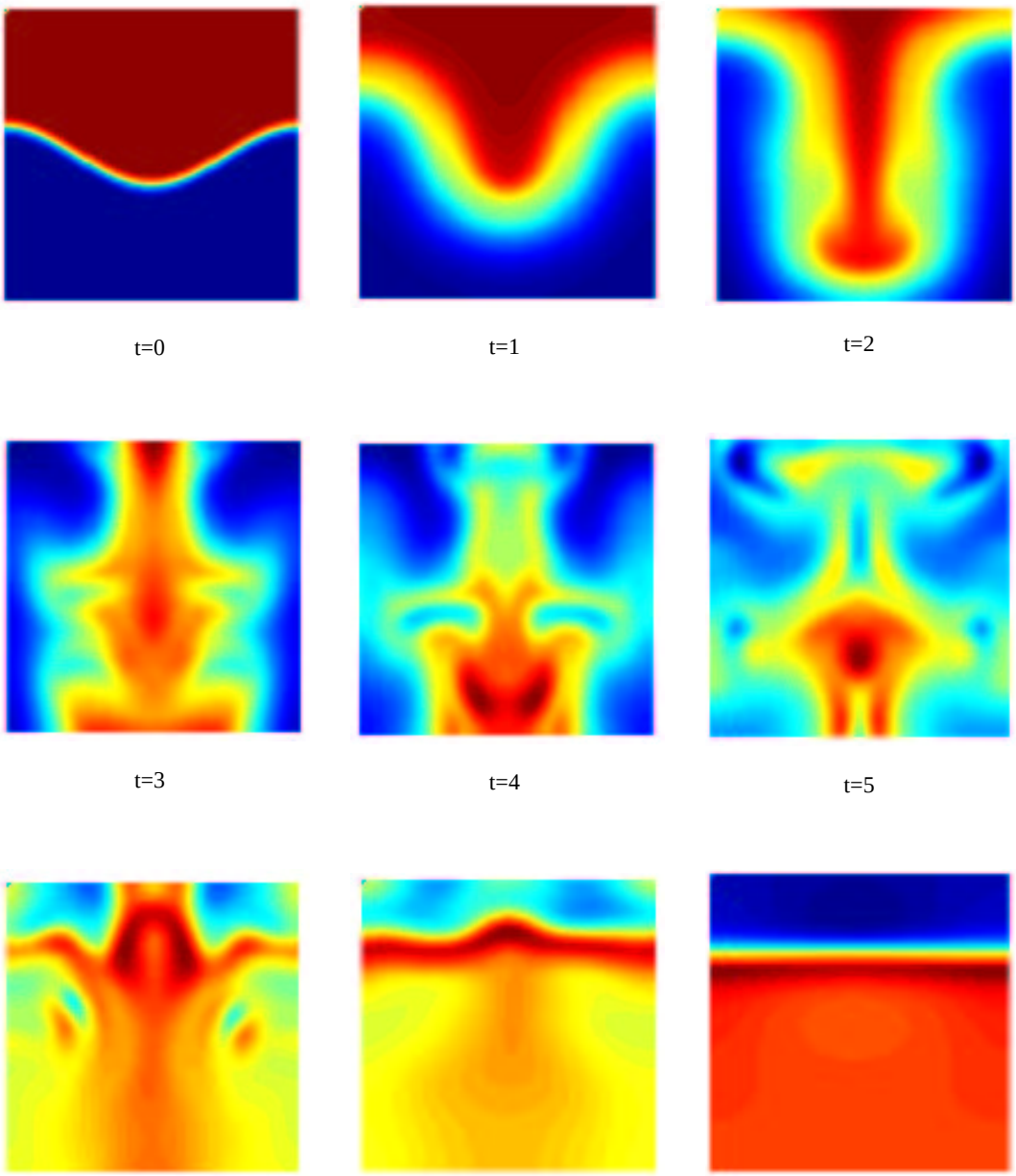
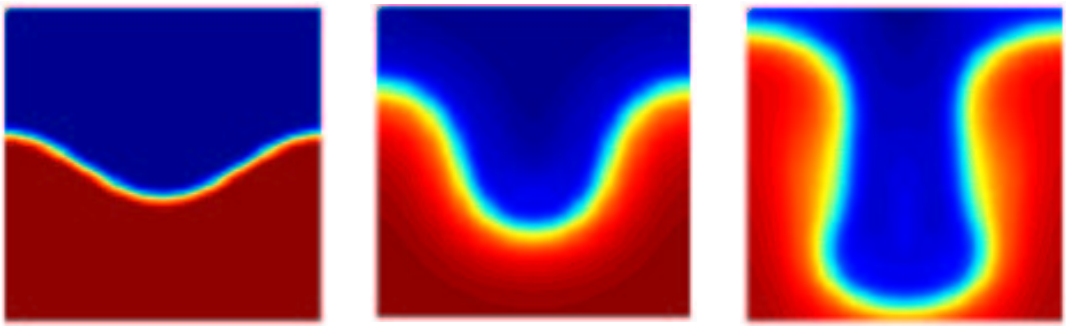
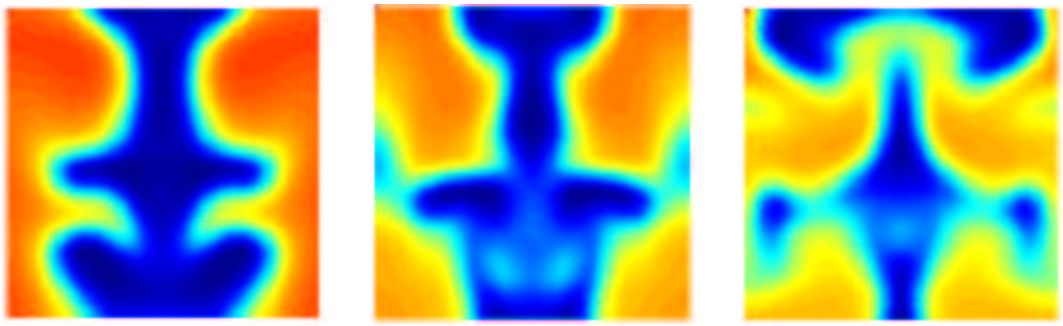


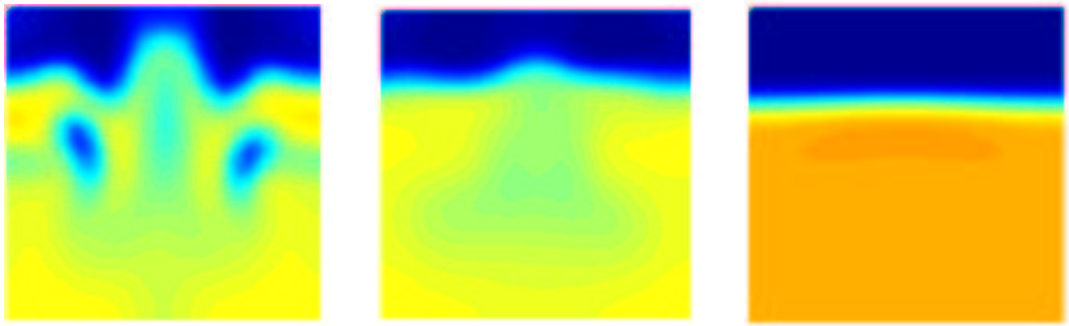
Figure 7.10: Evolution of concentration of fluid II.



t=0 t=1 t=2



t=3 t=4 t=5



t=6 t=7 t=50

Figure 7.11: Evolution of concentration of fluid III.

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