

# Numerical simulation of the three-dimensional Rayleigh–Taylor instability



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## ABSTRACT

The Rayleigh–Taylor instability is a fundamental instability of an interface between two fluids of different densities, which occurs when the light fluid is pushing the heavy fluid. During the nonlinear stages, the growth of the Rayleigh–Taylor instability is greatly affected by three-dimensional effects. To investigate three-dimensional effects on the Rayleigh–Taylor instability, we introduce a new method of computation of the flow of two incompressible and immiscible fluids and implement a time-dependent pressure boundary condition that relates to a time-dependent density field at the domain boundary. Through numerical examples, we observe the two-layer roll-up phenomenon of the heavy fluid, which does not occur in the two-dimensional case. And by studying the positions of the bubble front, spike tip, and saddle point, we show that the three-dimensional Rayleigh–Taylor instability exhibits a stronger dependence on the density ratio than on the Reynolds number. Finally, we perform a long time three-dimensional simulation resulting in an equilibrium state.

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## 1. Introduction

The Rayleigh–Taylor instability (RTI) is a fundamental instability of an interface between two fluids of different densities, which occurs when a heavy fluid is superposed over a light fluid in a gravitational field or when a hydrodynamic instability occurs in any accelerating fluid system in which the density and pressure gradients have opposite signs. For a fluid in a gravitational field, the RTI was first introduced by Rayleigh [1] and later applied in considering all accelerated fluids by Taylor [2]. The Rayleigh–Taylor instability has been applied in considering a wide range of problems such as inertial confinement fusion [3–6], supernova explosion [7,8] and remnants [9,10], atmospheric physics [11], geophysics [12], and oceanography [13].

The growth of the RTI can be roughly divided into four stages [14]. In the first stage, the amplitude  $h$  of the perturbation is much smaller than the wavelength  $\lambda$ . The linear stability theory is valid and shows that the amplitude grows exponentially with time [2]:

$$h = h_0 e^{\alpha t},$$

where  $h_0$  is the initial amplitude,  $\alpha$  is the growth rate, and  $t$  is the time. The growth rate depends on the density ratio ( $\rho_H/\rho_L$ , or Atwood number  $At = (\rho_H - \rho_L)/(\rho_H + \rho_L)$ , where  $\rho_H$  and  $\rho_L$  are the densities of the heavy and light fluids, respectively), the surface tension, the viscosity, and the compressibility [14]. When the amplitude grows to a size of order  $0.1\lambda$  to  $0.4\lambda$ , substantial deviations from the linear theory are observed and the RTI evolves into the second (nonlinear) stage. During the

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second stage, the light fluid rises into the heavy fluid in the form of bubbles and the heavy fluid falls into the light fluid in the form of spikes. In the third stage, the nonlinearity becomes much stronger. The Kelvin–Helmholtz instability [15] occurs due to a velocity difference across the interface between two fluids and a roll-up of vortices forms a mushroom-type shape of the spikes. Also, there is bubble amalgamation, in which large bubbles absorb smaller ones and large bubbles grow larger and move faster. In the final stage, the RTI evolves into turbulent or chaotic mixing.

The first two stages can be dealt with by the analytic and quasi-analytic methods [15]. The behavior during the late stages is mainly studied numerically. Although there have been many numerical studies [16–26], the nonlinear evolution of the three-dimensional RTI in the late stages, which results from different dimensionless parameters or Atwood numbers, has not been well documented and, furthermore, to the best of the authors' knowledge, numerical simulations were stopped well before the fluid system reached an equilibrium state. The purpose of this paper is to investigate the late stage evolution of the three-dimensional RTI of two fluids and to perform a long time three-dimensional simulation resulting in an equilibrium state.

In this paper, direct numerical simulations of the three-dimensional RTI are carried out using a phase-field method. The main idea of the method is to treat the interface between two fluids as a thin mixing layer across which physical properties vary steeply but continuously. The method avoids a direct tracking of the interface and produces the correct interfacial tension from the mixing layer free energy. The properties and evolution of the mixing layer are governed by an order parameter  $\phi$  (a phase-field variable) that obeys the Cahn–Hilliard equation [27]. The Cahn–Hilliard equation has been extensively studied using finite element methods [28–32], finite difference algorithms [33–40], spectral methods [41,42], and collocation techniques [43,44] based on Legendre and Chebyshev polynomials [45]. Recently, Dehghan and Mirzaei [46] applied a numerical method based on the boundary integral equation and dual reciprocity methods using radial basis functions [47,48].

The governing equations for two incompressible and immiscible fluids are the Navier–Stokes–Cahn–Hilliard equations [49–64]:

$$\rho(\phi) \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \frac{1}{Re} \Delta \mathbf{u} + \frac{\rho(\phi)}{Fr^2} \mathbf{g}, \tag{1}$$

$$\nabla \cdot \mathbf{u} = 0, \tag{2}$$

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{u}) = \frac{1}{Pe} \Delta \mu, \tag{3}$$

$$\mu = f(\phi) - \epsilon^2 \Delta \phi, \tag{4}$$

where  $\mathbf{u}$  is the velocity,  $p$  is the pressure,  $\rho(\phi) = (\rho_H(1 + \phi)/2 + \rho_L(1 - \phi)/2)\rho_c$  is the variable density,  $\mathbf{g} = (0, 0, -1)$  is the gravitational direction, and  $\mu$  is the generalized chemical potential.  $f(\phi) = \phi^3 - \phi$  and  $\epsilon$  are redefined according to the scaling. The dimensionless parameters are the Reynolds number,  $Re = \rho_c U_c L_c / \eta$ , the Froude number,  $Fr = U_c / \sqrt{g L_c}$ , and the Péclet number,  $Pe = U_c L_c / (M \mu_c)$ . Here, the subscript 'c' indicates characteristic values used to make the governing equations dimensionless,  $\eta$  is the viscosity,  $g$  is the gravitational acceleration, and  $M$  is the mobility. In this paper, the effect of the surface tension is neglected. We note that even though our phase-field method can deal with the variable viscosity case straightforwardly, we focus on the viscosity matched case. When the densities of two incompressible fluids are different, the incompressible condition (2) is no longer valid in the mixed region of the two incompressible fluids despite each fluid being incompressible. Such fluids are referred to as quasi-incompressible in Ref. [65]. In recent work [66], the authors discussed this issue and formulated a pair of phase-field models that conserve mass, momentum, and total volume for each individual phase of two fluids.

This paper is organized as follows. In Section 2, we give a numerical solution with linear and nonlinear multigrid methods [67,68]. The pressure boundary condition which allows long time simulation will also be addressed in this section. Numerical results for the three-dimensional RTI are presented in Section 3. In Section 4, conclusions are drawn.

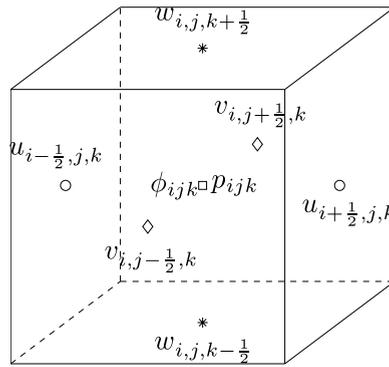
## 2. A numerical solution

The solution of large systems of equations resulting from discretization of the governing equations (1)–(4) is very costly, especially in three dimensions. An efficient approximation can be obtained by decoupling the solution of the momentum equations from the solution of the continuity equation by a projection method [69–74].

Let a three-dimensional computational domain be partitioned in Cartesian geometry into a uniform mesh with mesh spacing  $h$ . The center of each cell,  $\Omega_{ijk}$ , is located at  $(x_i, y_j, z_k) = ((i - 0.5)h, (j - 0.5)h, (k - 0.5)h)$  for  $i = 1, \dots, N_x, j = 1, \dots, N_y$ , and  $k = 1, \dots, N_z$ .  $N_x, N_y$ , and  $N_z$  are the numbers of cells in the  $x$ -,  $y$ -, and  $z$ -directions, respectively. Cell vertices are located at  $(x_{i+\frac{1}{2}}, y_{j+\frac{1}{2}}, z_{k+\frac{1}{2}}) = (ih, jh, kh)$ . In this paper, the fluid variables are defined on a staggered marker-and-cell (MAC) mesh introduced by Harlow and Welch [75]; that is, pressures and phase fields are stored at cell centers and velocities at cell faces (see Fig. 1).

Let  $\Delta t$  be the time step and  $n$  be the time step index. At the beginning of each time step, given  $\mathbf{u}^n$  and  $\phi^n$ , we want to find  $\mathbf{u}^{n+1}$ ,  $p^{n+1}$ , and  $\phi^{n+1}$  which solve the following temporal discretization of Eqs. (1)–(4):

$$\rho^n \frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = -\rho^n (\mathbf{u} \cdot \nabla \mathbf{u})^n - \nabla_d p^{n+1} + \frac{1}{Re} \Delta_d \mathbf{u}^n + \frac{\rho^n}{Fr^2} \mathbf{g},$$



**Fig. 1.** Location of the fluid variables on a MAC mesh cell. Velocities are defined at the cell faces while pressures and phase fields are defined at the cell centers.

$$\nabla_d \cdot \mathbf{u}^{n+1} = 0,$$

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = -\nabla_d \cdot (\phi \mathbf{u})^n + \frac{1}{Pe} \Delta_d v^{n+1} - \frac{1}{Pe} \Delta_d \phi^n, \tag{5}$$

$$v^{n+1} = (\phi^{n+1})^3 - \epsilon^2 \Delta_d \phi^{n+1}, \tag{6}$$

where  $\rho^n = \rho(\phi^n)$ . The outline of the main procedures in one time step is as follows.

*Step 1.* Initialize  $\phi^0$  to be the locally equilibrated composition profile and  $\mathbf{u}^0$  to be the divergence-free velocity field.

*Step 2.* Solve for an intermediate velocity field,  $\tilde{\mathbf{u}}$ , which generally does not satisfy the continuity equation, without the pressure gradient:

$$\frac{\tilde{\mathbf{u}} - \mathbf{u}^n}{\Delta t} = -(\mathbf{u} \cdot \nabla_d \mathbf{u})^n + \frac{1}{\rho^n Re} \Delta_d \mathbf{u}^n + \frac{1}{Fr^2} \mathbf{g},$$

where the convective term,  $(\mathbf{u} \cdot \nabla_d \mathbf{u})^n$ , is computed using an upwind scheme [62,63].

Then, we solve the following equations for the advanced pressure field at the  $(n + 1)$ th time step:

$$\frac{\mathbf{u}^{n+1} - \tilde{\mathbf{u}}}{\Delta t} = -\frac{1}{\rho^n} \nabla_d p^{n+1}, \tag{7}$$

$$\nabla_d \cdot \mathbf{u}^{n+1} = 0. \tag{8}$$

Applying the divergence operator to Eq. (7), we find that Eq. (7) is equivalent to a Poisson equation for  $p^{n+1}$ :

$$\nabla_d \cdot \left( \frac{1}{\rho^n} \nabla_d p^{n+1} \right) = \frac{1}{\Delta t} \nabla_d \cdot \tilde{\mathbf{u}}, \tag{9}$$

where we have made use of Eq. (8) and the terms are defined as follows:

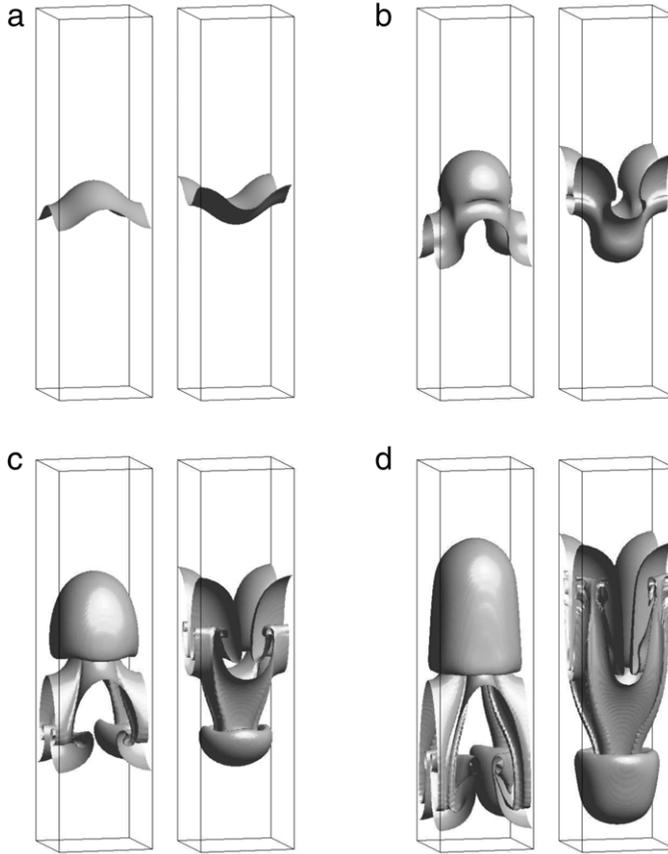
$$\begin{aligned} \nabla_d \cdot \left( \frac{1}{\rho^n} \nabla_d p_{ijk}^{n+1} \right) &= \frac{\frac{1}{\rho^n} p_{i+1,j,k}^{n+1} + \frac{1}{\rho^n} p_{i-1,j,k}^{n+1} + \frac{1}{\rho^n} p_{i,j+1,k}^{n+1} + \frac{1}{\rho^n} p_{i,j-1,k}^{n+1}}{h^2} \\ &\quad + \frac{\frac{1}{\rho^n} p_{i,j,k+\frac{1}{2}}^{n+1} + \frac{1}{\rho^n} p_{i,j,k-\frac{1}{2}}^{n+1}}{h^2} \\ &\quad - \frac{\frac{1}{\rho^n} \frac{1}{i+\frac{1}{2},j,k} + \frac{1}{\rho^n} \frac{1}{i-\frac{1}{2},j,k} + \frac{1}{\rho^n} \frac{1}{i,j+\frac{1}{2},k} + \frac{1}{\rho^n} \frac{1}{i,j-\frac{1}{2},k} + \frac{1}{\rho^n} \frac{1}{i,j,k+\frac{1}{2}} + \frac{1}{\rho^n} \frac{1}{i,j,k-\frac{1}{2}}}{h^2} p_{ijk}^{n+1}, \\ \nabla_d \cdot \tilde{\mathbf{u}}_{ijk} &= \frac{\tilde{u}_{i+\frac{1}{2},j,k} - \tilde{u}_{i-\frac{1}{2},j,k}}{h} + \frac{\tilde{v}_{i,j+\frac{1}{2},k} - \tilde{v}_{i,j-\frac{1}{2},k}}{h} + \frac{\tilde{w}_{i,j,k+\frac{1}{2}} - \tilde{w}_{i,j,k-\frac{1}{2}}}{h}, \end{aligned}$$

where  $\rho^n_{i+\frac{1}{2},j,k} = (\rho^n_{i+1,j,k} + \rho^n_{ijk})/2$  and the other terms are similarly defined.

The boundary condition for the pressure [62] is

$$\mathbf{n} \cdot \nabla_d p^{n+1} = \mathbf{n} \cdot \left( -\rho^n \frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} - \rho^n (\mathbf{u} \cdot \nabla_d \mathbf{u})^n + \frac{1}{Re} \Delta_d \mathbf{u}^n + \frac{\rho^n}{Fr^2} \mathbf{g} \right),$$

where  $\mathbf{n}$  is the unit vector normal to the domain boundary.



**Fig. 2.** Evolution of the interface at (a)  $t = 1.0$ , (b)  $t = 2.0$ , (c)  $t = 3.0$ , and (d)  $t = 4.0$ . The Atwood number is 0.5 and the Reynolds number is 1024. The interface is viewed from the heavy-fluid side (left column) and from the light-fluid side (right column). The interfaces in the left column are shifted 0.5 in both  $x$ - and  $y$ -directions for a better view of the bubble.

In our application of the phase-field method to the three-dimensional RTI, we will use periodic boundary conditions at the four sides and no slip boundary conditions at the top and bottom walls. Therefore,

$$\mathbf{n} \cdot \nabla_d p^{n+1} = \mathbf{n} \cdot \frac{\rho^n}{Fr^2} \mathbf{g}, \quad \text{i.e., } \frac{\partial p^{n+1}}{\partial z} = -\frac{\rho^n}{Fr^2} \text{ at } z = 0 \text{ and } z = L_z.$$

The resulting linear system of Eq. (9) is solved by a fast solver, such as a linear multigrid method [67]. Also, a Gauss–Seidel relaxation scheme is used as the smoother in the multigrid method. Then, the divergence-free velocities are defined by

$$\mathbf{u}^{n+1} = \tilde{\mathbf{u}} - \frac{\Delta t}{\rho^n} \nabla_d p^{n+1}.$$

*Step 3.* Update the phase field  $\phi^n$  to  $\phi^{n+1}$ . We implement an unconditionally gradient stable scheme in Eqs. (5) and (6) with a nonlinear multigrid method [67]. For a detailed description of the numerical method used in solving Eqs. (5) and (6), please refer to Refs. [38,76].

Since we are interested in a long time simulation, mass conservation is an important factor. Therefore, we use a conservative discretization of the convective part of the phase field Eq. (5):

$$\begin{aligned} ((\phi u)_x + (\phi v)_y + (\phi w)_z)_{ijk}^n &= \frac{u_{i+\frac{1}{2},j,k}^n (\phi_{i+1,j,k}^n + \phi_{ijk}^n) - u_{i-\frac{1}{2},j,k}^n (\phi_{ijk}^n + \phi_{i-1,j,k}^n)}{2h} \\ &+ \frac{v_{i,j+\frac{1}{2},k}^n (\phi_{i,j+1,k}^n + \phi_{ijk}^n) - v_{i,j-\frac{1}{2},k}^n (\phi_{ijk}^n + \phi_{i,j-1,k}^n)}{2h} \\ &+ \frac{w_{i,j,k+\frac{1}{2}}^n (\phi_{i,j,k+1}^n + \phi_{ijk}^n) - w_{i,j,k-\frac{1}{2}}^n (\phi_{ijk}^n + \phi_{i,j,k-1}^n)}{2h}. \end{aligned}$$

These complete one time step.

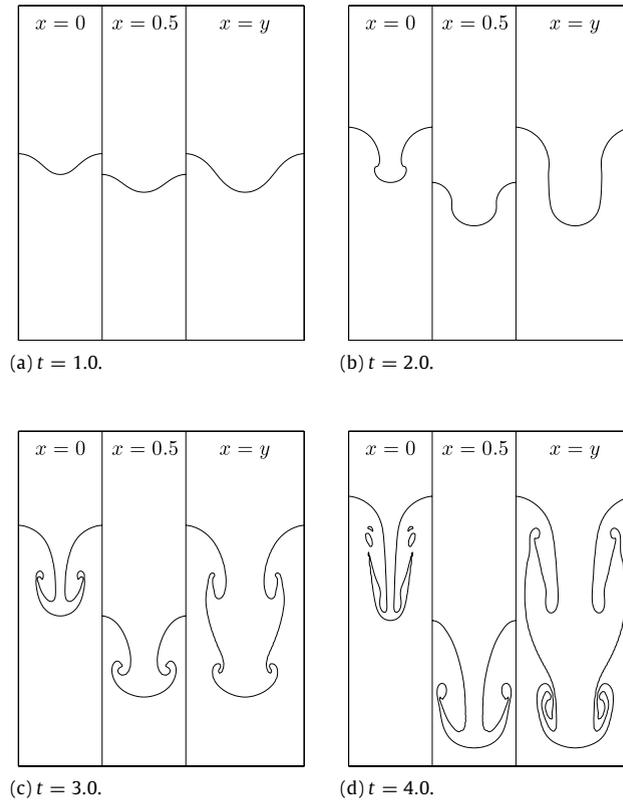


Fig. 3. Cross-sectional views of the interface at three vertical planes,  $x = 0$ ,  $x = 0.5$ , and  $x = y$ . Times are shown below each figure.

### 3. Numerical results

In this section, we simulate the three-dimensional RTI in a rectangular box with a square horizontal cross-section. In the previous work of He et al. [22], similar numerical experiments were performed using a lattice Boltzmann method. The height–width aspect ratio is fixed at 4:1. Unless otherwise specified, the initial condition is

$$\phi(x, y, z, 0) = \tanh\left(\frac{z - 2 - 0.05(\cos(2\pi x) + \cos(2\pi y))}{\sqrt{2}\epsilon}\right)$$

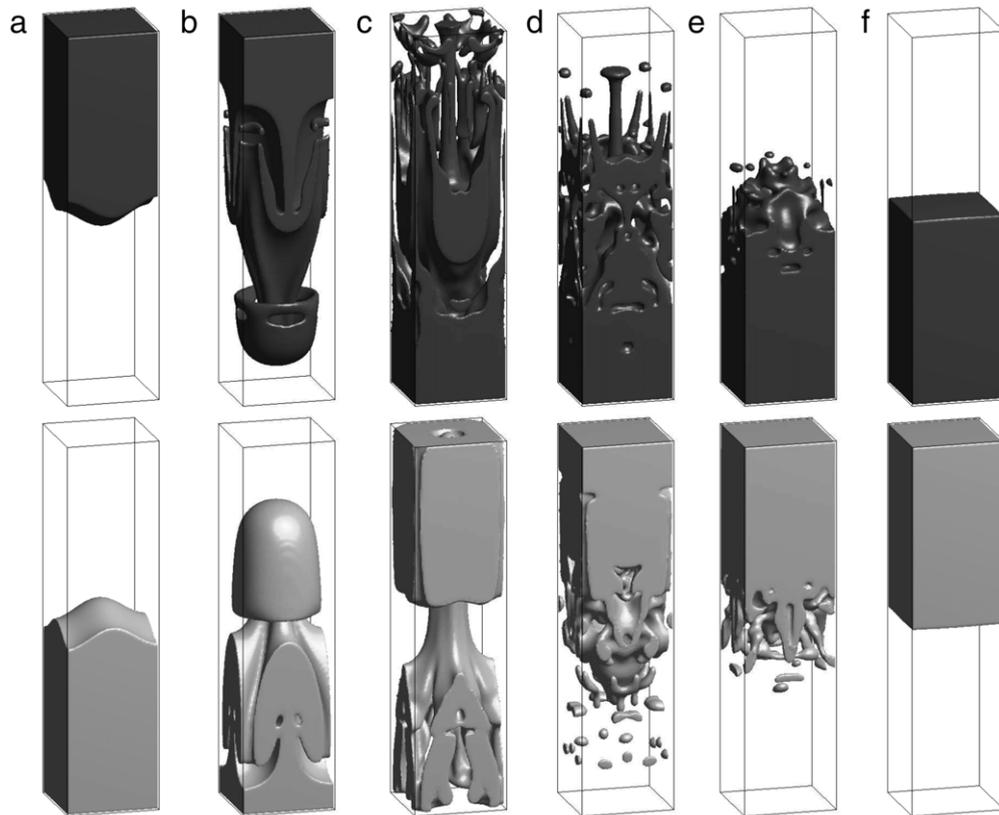
on the computational domain  $\Omega = (0, 1) \times (0, 1) \times (0, 4)$ .

#### 3.1. Three-dimensional Rayleigh–Taylor instability

The evolution of the interface in the three-dimensional RTI is shown in Fig. 2. Left and right columns in each subfigure show two different views of the interface from the heavy-fluid side and the light-fluid side, respectively. Here, the Atwood number is 0.5 and the Reynolds number is 1024. And we use  $h = 1/128$  (a  $128 \times 128 \times 512$  grid),  $\Delta t = 0.001$ ,  $\epsilon = 0.01$ , and  $Pe = 100/\epsilon$ . During the early stages, the interface grows nearly symmetrically up and down and remains rather simple (see Fig. 2(a)). But, as time goes by, it becomes more complicated and spikes of the heavy fluid first form near the middle of the four sides of the computational domain (see Fig. 2(b)). The roll-up at the edge of the spike starts at a later time (see Fig. 2(c)). At  $t = 4.0$ , these roll-ups are stretched into two extra layers of the heavy fluid folded upward (see Fig. 2(d)). This two-layer roll-up phenomenon is a unique feature of the three-dimensional RTI. Fig. 3 shows cross-sectional views of the interface at three vertical planes,  $x = 0$ ,  $x = 0.5$ , and  $x = y$ . The interfaces in the  $x = 0$  and  $x = 0.5$  planes look like those in the two-dimensional RTI. However, the interface in the  $x = y$  plane is quite different. In this plane, we can see clearly the two-layer roll-up phenomenon. These results are in qualitative agreement with the previous computations of Li et al. [21] and He et al. [22].

#### 3.2. Long time evolution of the three-dimensional Rayleigh–Taylor instability

Owing to the pressure boundary treatment mentioned in Section 2, we can perform long time evolution resulting in an equilibrium state. The Atwood number is 0.5 and the Reynolds number is 3000. And we use  $h = 1/64$  (a  $64 \times 64 \times 256$



**Fig. 4.** Long time evolution of the three-dimensional Rayleigh–Taylor instability at (a)  $t = 0$ , (b)  $t = 3.53$ , (c)  $t = 7.07$ , (d)  $t = 14.14$ , (e)  $t = 17.67$ , and (f)  $t = 70.7$ . Top and bottom rows show two different views of the interface from the light-fluid side and the heavy-fluid side, respectively.

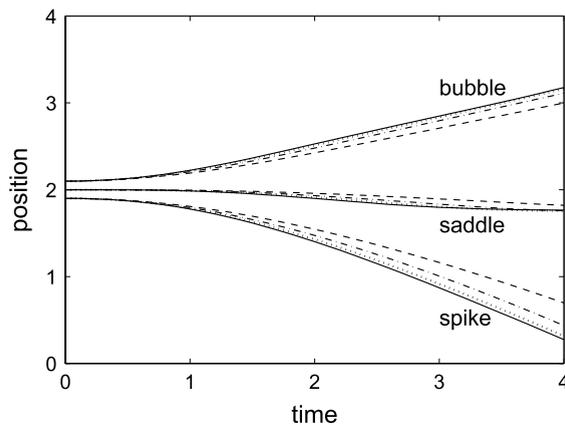
grid),  $\Delta t = 0.001\sqrt{2}$ ,  $\epsilon = 0.01\sqrt{2}$ , and  $Pe = 1/\epsilon$ . The evolution of the interface is shown in Fig. 4. At time  $t = 70.7$ , the heavy fluid falls down and the light fluid rises up completely.

### 3.3. The effect of the Reynolds number

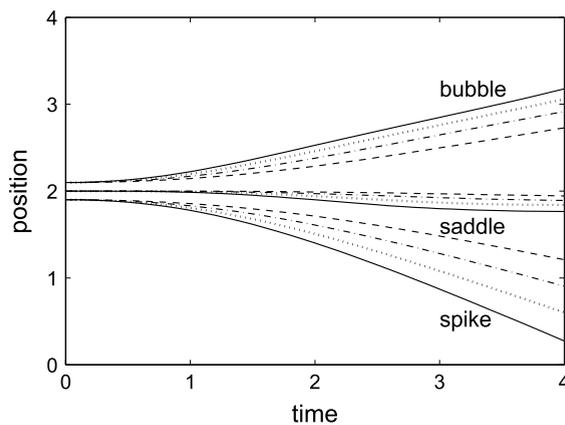
To investigate the effect of the Reynolds number on the three-dimensional RTI, we perform numerical simulations at a number of Reynolds numbers with the Atwood number fixed at 0.5. We use  $h = 1/128$  (a  $128 \times 128 \times 512$  grid),  $\Delta t = 0.001$ ,  $\epsilon = 0.01$ , and  $Pe = 1/\epsilon$ . Fig. 5 shows the positions of the bubble front, spike tip, and saddle point at different Reynolds numbers. For all Reynolds numbers, at later times, the bubble rises with a constant speed and the spike accelerates slightly. The saddle points move downward as time increases, but the movement is rather slow compared to those of the bubble and spike. Also, we observe that a decrease in the Reynolds number delays the development of the RTI. This delay is larger for the spike than for the bubble and saddle points. The effect of the Reynolds number is obvious at low Reynolds numbers but becomes negligible for  $Re > 512$ .

### 3.4. The effect of the Atwood number

To study the effect of the Atwood number on the three-dimensional RTI, we perform numerical simulations at a number of Atwood numbers with the Reynolds number fixed at 1024. We use  $h = 1/128$  (a  $128 \times 128 \times 512$  grid),  $\Delta t = 0.001$ ,  $\epsilon = 0.01$ , and  $Pe = 1/\epsilon$ . Fig. 6 shows the positions of the bubble front, spike tip, and saddle point at different Atwood numbers. When the Atwood number is small (at  $At = 0.2$ ), the position change of the bubble front is almost the same as that of the spike tip. This means that the interface grows nearly symmetrically up and down. However, as the Atwood number increases, the position of the spike tip changes much more quickly than that of the bubble front and the symmetry of the initial structure becomes lost. From the results of Fig. 6, we see that the three-dimensional RTI exhibits a strong dependence on the Atwood number.



**Fig. 5.** Effect of the Reynolds number on the positions of the bubble front, spike tip, and saddle point. The Atwood number is fixed at 0.5. Solid, dotted, dash-dotted, and dashed lines show the results for  $Re = 1024, 512, 256,$  and  $128,$  respectively.



**Fig. 6.** Effect of the Atwood number on the positions of the bubble front, spike tip, and saddle point. The Reynolds number is fixed at 1024. Solid, dotted, dash-dotted, and dashed lines are the results of  $At = 0.5, 0.4, 0.3,$  and  $0.2,$  respectively.

#### 4. Conclusions

The three-dimensional RTI between two incompressible and immiscible fluids was studied using a phase field. During the early stages, the interface grows nearly symmetrically up and down and remains rather simple. During the late stages, the heavy fluid rolls up at both the saddle point and the spike tip due to the Kelvin–Helmholtz instability. As a result, we observed the two-layer roll-up phenomenon of the heavy fluid, which does not occur in the two-dimensional case. And we studied the positions of the bubble front, spike tip, and saddle point to investigate the effect of the Reynolds and Atwood numbers on the three-dimensional RTI. We showed that a decrease in the Reynolds or Atwood numbers delays the development of the RTI. Note that the three-dimensional RTI exhibits a stronger dependence on the Atwood number than on the Reynolds number. Finally, owing to the pressure boundary treatment, we were able to perform long time three-dimensional simulation resulting in an equilibrium state.

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