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A three-dimensional conservative Allen–Cahn model with a curvature-dependent Lagrange multiplier

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ABSTRACT

We propose a new three-dimensional (3D) conservative Allen–Cahn (CAC) model with a curvature-dependent Lagrange multiplier. The proposed model conserves the total mass and reduces unwanted curvature effects. It also keeps small structures and complex interface shapes better than conventional CAC models. We develop a simple numerical method that uses operator splitting, a Fourier spectral method, an exact solution for the reaction term, and a finite difference method for curvature calculation. The proposed method calculates curvature only near the interface to improve stability. We test the proposed model with several 3D examples such as multiple droplets, complex shapes, interface motion under a given velocity field, and a comparison with the Cahn–Hilliard model. The computational results show that the proposed model keeps the original shapes, conserves mass, and stays stable during the simulations. These numerical results show that the proposed model is a simple and effective method for 3D multiphase simulations.

1. Introduction

Phase-field methods are widely used to model problems that involve moving interfaces in science and engineering. These methods describe interfaces as thin transition layers and avoid tracking the interface explicitly. Because of this advantage, they are used in many problems such as topology optimization (Lai et al., 2025), crystal growth (Xie et al., 2025), and multiphase systems (Li et al., 2025; Xia et al., 2025). In some advanced works, the phase-field model was modified to construct complex solid geometries based on arbitrary point clouds (Fu et al., 2025; Gao et al., 2026). Among phase-field equations, the Allen–Cahn (AC) model is one of the most basic and well-known equations. The AC equation describes phase separation (Sohaib et al., 2025) and interface motion in binary systems (Lee et al., 2025). However, it does not conserve the total mass. Therefore, it is not suitable for problems where the total mass must remain constant.

To solve this problem, researchers proposed conservative Allen–Cahn (CAC) equations that use a Lagrange multiplier to keep the total mass constant over time. These equations are easier to compute than the Cahn–Hilliard (CH) model because they are second-order equations; however, the interface still evolves under mean curvature while the total mass remains constant, which is suitable in many physical cases because it helps smooth the interface and reduce energy (Liu et al., 2024). However, there are applications in which curvature-driven motion is not desirable. For example, in multiphase systems that contain structures of different sizes, small components may shrink and disappear due to their high curvature, even when such behavior is not physically relevant. In addition, in problems where the geometric features of the interface are important, they must be preserved. These effects limit the applicability

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of conventional CAC models in situations where both mass conservation and shape preservation are required (Sato & Koshimura, 2023). To reduce the local mass loss due to interfacial curvature, Su and Yang (2026) recently presented a ternary phase-field fluid system with curvature-dependent mobility, where the phase-field dynamics was suppressed according to interfacial curvature. To satisfy total mass conservation, the curvature-dependent mobility was only used in the CH-type equations. Furthermore, from a theoretical perspective, the spontaneous shrinkage of small structures in conventional multiphase models is governed by specific scaling laws, as comprehensively analyzed by Yue et al. (2007) for phase-field simulations. Similarly, for the conventional CAC model with a spatially constant Lagrange multiplier, asymptotic analysis demonstrates that the interface evolution follows volume-preserving mean curvature flow (Rubinstein & Sternberg, 1992). In Lee et al. (2020), the authors also implied that small structures will inevitably shrink when their radius falls below the critical threshold.

For these reasons, it is important to regulate the effect of curvature on interface motion. We introduce a curvature-dependent Lagrange multiplier in a three-dimensional (3D) CAC model. The proposed model controls the influence of curvature while preserving the total mass. As a result, it reduces undesired deformation and maintains the key geometric features of the interface. The proposed curvature-dependent method is a mathematical model. It is not based on classical thermodynamics. Traditional models produce mean curvature minus average mean curvature flow. In contrast, the proposed model reduces this motion. This method is useful for strong fluid flow and topology optimization because it keeps small shapes from disappearing under mean curvature minus average mean curvature flow. Kwak et al. (2022) presented a modified two-dimensional CAC model with a curvature-dependent term. This term controls curvature effects and preserves mass. Their model reduces the shrinkage of small structures and keeps the interface shape better than the standard CAC equation. Lee (2025) proposed a novel CAC model that preserves the zero-level interface during evolution while maintaining mass conservation. The model introduces variable mobility functions and a tailored correction term to prevent interface distortion caused by conventional adjustments. Xie et al. (2023) presented a modified phase-field equation that removes curvature effects, because such effects can cause excessive smoothing and degrade geometric features during evolution.

The organization of this article is as follows. In Section 2, we present the proposed CAC model and the numerical algorithm used to solve the model. In Section 3, we provide several computational tests to evaluate the performance of the geometric-feature-preserving property. Finally, Section 4 concludes the paper.

2. Curvature-dependent CAC model and numerical method

2.1. Conventional CAC models

Several forms of CAC equations have been developed to enforce mass conservation in the classical AC equation. We introduce two commonly used CAC equations that serve as reference models. The first CAC model (Rubinstein & Sternberg, 1992) introduces a spatially constant Lagrange multiplier to preserve the total mass. It is written as

$$\partial_t \phi = -\frac{F'(\phi)}{\epsilon^2} + \Delta \phi + \lambda_1(t), \quad (1)$$

where the Lagrange multiplier

$$\lambda_1(t) = \frac{1}{\epsilon^2 |\Omega|} \int_{\Omega} F'(\phi) d\Omega,$$

is obtained from the mass conservation condition. This model satisfies the mass conservation property. The second CAC equation includes a nonlocal correction term that depends on the phase variable, see Hwang et al. (2026) and references therein. It is given by

$$\partial_t \phi = -\frac{F'(\phi)}{\epsilon^2} + \Delta \phi + \lambda_2(t) \sqrt{2F(\phi)},$$

where the Lagrange multiplier

$$\lambda_2(t) = \frac{\int_{\Omega} F'(\phi) d\Omega}{\epsilon^2 \int_{\Omega} \sqrt{2F(\phi)} d\Omega},$$

is determined by the mass conservation condition so that the total mass is conserved.

2.2. Curvature-dependent CAC equation

Let $\Omega \subset \mathbb{R}^3$ be a computational domain and let $\phi = \phi(x, y, z, t)$ denote the phase-field function and $F(\phi) = 0.25(\phi^2 - 1)^2$. We consider a 3D CAC equation in which the Lagrange multiplier depends on the curvature.

$$\partial_t \phi = -\frac{F'(\phi)}{\epsilon^2} + \Delta \phi + \lambda(t) \kappa(\phi) \sqrt{2F(\phi)}. \quad (2)$$

Here, $\lambda(t)$ is a time-dependent Lagrange multiplier and $\kappa(\phi)$ denotes the curvature associated with the phase-field variable, defined by

$$\kappa(\phi) = \nabla \cdot \left(\frac{\nabla \phi}{|\nabla \phi|} \right).$$

The multiplier $\lambda(t)$ is determined so that the total mass of the phase-field variable is conserved. The explicit form of $\lambda(t)$ is given by

$$\lambda(t) = \frac{\int_{\Omega} F'(\phi) d\Omega}{\epsilon^2 \int_{\Omega} \kappa(\phi) \sqrt{2F(\phi)} d\Omega}.$$

The proposed Eq. (2) preserves the total mass of the solution. Let the total mass be defined as

$$\mathcal{M}(t) = \int_{\Omega} \phi(x, y, z, t) d\Omega.$$

We take the time derivative of $\mathcal{M}(t)$

$$\frac{d\mathcal{M}(t)}{dt} = \int_{\Omega} \partial_t \phi d\Omega. \quad (3)$$

We substitute the proposed Eq. (2) into Eq. (3)

$$\frac{d\mathcal{M}(t)}{dt} = \int_{\Omega} \left(-\frac{F'(\phi)}{\epsilon^2} + \Delta\phi + \lambda(t)\kappa(\phi)\sqrt{2F(\phi)} \right) d\Omega.$$

The divergence theorem gives $\int_{\Omega} \Delta\phi d\Omega = \int_{\partial\Omega} \mathbf{n} \cdot \nabla\phi ds$. We assume the zero Neumann boundary condition $\mathbf{n} \cdot \nabla\phi = 0$ on $\partial\Omega$. Therefore, $\int_{\Omega} \Delta\phi d\Omega = 0$. Hence,

$$\frac{d\mathcal{M}(t)}{dt} = -\frac{1}{\epsilon^2} \int_{\Omega} F'(\phi) d\Omega + \lambda(t) \int_{\Omega} \kappa(\phi) \sqrt{2F(\phi)} d\Omega.$$

From the definition of $\lambda(t)$, we obtain

$$\frac{d\mathcal{M}(t)}{dt} = 0.$$

Thus, the proposed Eq. (2) preserves the total mass

$$\int_{\Omega} \phi(x, y, z, t) d\Omega = \int_{\Omega} \phi(x, y, z, 0) d\Omega.$$

Remark 1. The factor $\sqrt{2F(\phi)}$ is closely related to the equilibrium profile of the AC equation. Consider a moving interface with the profile

$$\phi(\mathbf{x}, t) = \tanh\left(\frac{d(\mathbf{x}, t)}{\sqrt{2\epsilon}}\right),$$

where $d(\mathbf{x}, t)$ is a signed distance function. Since

$$\sqrt{2F(\phi)} = \frac{1 - \phi^2}{\sqrt{2}},$$

the time derivative of the profile satisfies

$$\phi_t = \frac{d_t}{\epsilon} \sqrt{2F(\phi)}.$$

Thus, a source term proportional to $\sqrt{2F(\phi)}$ is consistent with the normal motion of a tanh-shaped diffuse interface (Wang et al., 2021). In the proposed model, the coefficient $\lambda(t)\kappa(\phi)$ controls this motion according to the local curvature.

The proposed correction also suppresses the leading-order curvature motion of the AC equation. For a well-prepared tanh profile with $|\nabla d| = 1$, we formally obtain

$$\Delta\phi - \frac{F'(\phi)}{\epsilon^2} \approx \frac{\kappa(\phi)}{\epsilon} \sqrt{2F(\phi)}$$

near the interface. Under the zero Neumann boundary condition, integration over Ω gives

$$\frac{1}{\epsilon^2} \int_{\Omega} F'(\phi) d\Omega \approx -\frac{1}{\epsilon} \int_{\Omega} \kappa(\phi) \sqrt{2F(\phi)} d\Omega.$$

Therefore, the mass-conserving Lagrange multiplier formally satisfies $\lambda(t) \approx -1/\epsilon$, provided that its denominator is nonzero. Hence, the correction term cancels the leading-order curvature contribution of the AC equation. The factor $\sqrt{2F(\phi)}$ remains consistent with the tanh-shaped transition layer, while the global multiplier preserves the total mass. This formal argument explains the shape-preserving and mass-conserving mechanisms of the proposed model.

It is important to note a theoretical distinction regarding the maximum principle. A primary advantage of the standard AC equation over the CH equation is that it strictly satisfies the maximum principle. However, the nonlocal Lagrange multiplier for mass conservation usually does not keep this property. Recent studies proposed numerical methods that keep the maximum principle for the standard CAC equation (Choi & Kim, 2023). However, it is still difficult to keep the maximum principle for a CAC equation with a curvature-dependent multiplier.

2.3. Numerical scheme

Let the computational domain be $\Omega = (L_x, R_x) \times (L_y, R_y) \times (L_z, R_z)$. We use a uniform cell-centered grid with N_x , N_y , and N_z grid points corresponding to the x -, y -, and z -directions. The grid spacing is $h = (R_x - L_x)/N_x = (R_y - L_y)/N_y = (R_z - L_z)/N_z$. The grid points are defined as $(x_i, y_j, z_k) = (L_x + (i-1/2)h, L_y + (j-1/2)h, L_z + (k-1/2)h)$ for $1 \leq i \leq N_x$, $1 \leq j \leq N_y$, and $1 \leq k \leq N_z$. Let ϕ_{ijk}^n denote the numerical approximation of $\phi(x_i, y_j, z_k, n\Delta t)$, where Δt is the time step size. We apply an operator splitting method (OSM) to separate the original equation into three subproblems:

$$\partial_t \phi = \Delta \phi, \quad (4)$$

$$\partial_t \phi = -\frac{F'(\phi)}{e^2}, \quad (5)$$

$$\partial_t \phi = \lambda(t)\kappa(\phi)\sqrt{2F(\phi)}. \quad (6)$$

These subproblems correspond to diffusion, reaction, and curvature correction, respectively. We solve Eqs. (4)–(6) sequentially within each time step.

We solve Eq. (4) with a Fourier spectral method based on the discrete cosine transform (DCT). Let $p = 1, \dots, N_x$, $q = 1, \dots, N_y$, and $r = 1, \dots, N_z$ denote the transform indices associated with the x , y , and z coordinates. We define the spectral wave numbers by $\xi_p = \pi(p-1)/(R_x - L_x)$, $\eta_q = \pi(q-1)/(R_y - L_y)$, and $\zeta_r = \pi(r-1)/(R_z - L_z)$. The DCT of the numerical solution ϕ_{ijk}^n is defined as

$$\hat{\phi}_{pqr}^n = \alpha_p \beta_q \gamma_r \sum_{i,j,k} \phi_{ijk}^n \cos(\xi_p(x_i - L_x)) \cos(\eta_q(y_j - L_y)) \cos(\zeta_r(z_k - L_z)). \quad (7)$$

The normalization coefficients are

$$\alpha_p = \begin{cases} \sqrt{\frac{1}{N_x}}, & p = 1, \\ \sqrt{\frac{2}{N_x}}, & 2 \leq p \leq N_x, \end{cases} \quad \beta_q = \begin{cases} \sqrt{\frac{1}{N_y}}, & q = 1, \\ \sqrt{\frac{2}{N_y}}, & 2 \leq q \leq N_y, \end{cases} \quad \gamma_r = \begin{cases} \sqrt{\frac{1}{N_z}}, & r = 1, \\ \sqrt{\frac{2}{N_z}}, & 2 \leq r \leq N_z. \end{cases}$$

The inverse discrete cosine transform (IDCT) is

$$\phi_{ijk}^n = \sum_{p,q,r} \alpha_p \beta_q \gamma_r \hat{\phi}_{pqr}^n \cos(\xi_p(x_i - L_x)) \cos(\eta_q(y_j - L_y)) \cos(\zeta_r(z_k - L_z)). \quad (8)$$

The Laplacian of the cosine basis functions satisfies

$$\begin{aligned} \Delta [\cos(\xi_p(x - L_x)) \cos(\eta_q(y - L_y)) \cos(\zeta_r(z - L_z))] \\ = -(\xi_p^2 + \eta_q^2 + \zeta_r^2) \cos(\xi_p(x - L_x)) \cos(\eta_q(y - L_y)) \cos(\zeta_r(z - L_z)). \end{aligned}$$

Therefore, in Eq. (4) the transformed equation is

$$\partial_t \hat{\phi}_{pqr} = -(\xi_p^2 + \eta_q^2 + \zeta_r^2) \hat{\phi}_{pqr}. \quad (9)$$

Eq. (9) has the exact solution

$$\hat{\phi}_{pqr}(t) = \hat{\phi}_{pqr}(0) e^{-(\xi_p^2 + \eta_q^2 + \zeta_r^2)t}.$$

Therefore, the exact solution in spectral space after one time step is

$$\hat{\phi}_{pqr}^{n+1,1} = \hat{\phi}_{pqr}^n e^{-\Delta t(\xi_p^2 + \eta_q^2 + \zeta_r^2)}.$$

Finally, the solution in physical space is obtained through the IDCT:

$$\phi_{ijk}^{n+1,1} = \sum_{p,q,r} \alpha_p \beta_q \gamma_r \hat{\phi}_{pqr}^{n+1,1} \cos(\xi_p(x_i - L_x)) \cos(\eta_q(y_j - L_y)) \cos(\zeta_r(z_k - L_z)).$$

Second, we consider Eq. (5). Because $F'(\phi) = \phi(\phi^2 - 1)$, Eq. (5) can be rewritten as

$$\partial_t \phi = -\frac{1}{e^2} \phi(\phi^2 - 1).$$

This ordinary differential equation has an analytic solution. The solution after one time step Δt is

$$\phi_{ijk}^{n+1,2} = \frac{\phi_{ijk}^{n+1,1}}{\sqrt{e^{-\frac{2\Delta t}{e^2}} + \left(\phi_{ijk}^{n+1,1}\right)^2 \left(1 - e^{-\frac{2\Delta t}{e^2}}\right)}}.$$

Third, we consider Eq. (6). We discretize Eq. (6) as

$$\frac{\phi_{ijk}^{n+1} - \phi_{ijk}^{n+1,2}}{\Delta t} = \gamma^{n+1,2} \kappa_{ijk}^{n+1,2} \sqrt{2F(\phi_{ijk}^{n+1,2})}. \quad (10)$$

From Eq. (10), we obtain

$$\phi_{ijk}^{n+1} = \phi_{ijk}^{n+1,2} + \Delta t \gamma^{n+1,2} \kappa_{ijk}^{n+1,2} \sqrt{2F(\phi_{ijk}^{n+1,2})}. \quad (11)$$

The scheme preserves the total mass. Thus we impose the discrete mass conservation condition

$$\sum_{i,j,k} \phi_{ijk}^{n+1} = \sum_{i,j,k} \phi_{ijk}^0. \quad (12)$$

Substituting Eq. (11) into Eq. (12) gives

$$\sum_{i,j,k} \left(\phi_{ijk}^{n+1,2} + \Delta t \gamma^{n+1,2} \kappa_{ijk}^{n+1,2} \sqrt{2F(\phi_{ijk}^{n+1,2})} \right) = \sum_{i,j,k} \phi_{ijk}^0. \quad (13)$$

From Eq. (13), the discrete Lagrange multiplier is

$$\gamma^{n+1,2} = \frac{\sum_{i,j,k} (\phi_{ijk}^0 - \phi_{ijk}^{n+1,2})}{\Delta t \sum_{i,j,k} \kappa_{ijk}^{n+1,2} \sqrt{2F(\phi_{ijk}^{n+1,2})}}.$$

After computing $\gamma^{n+1,2}$, we obtain the updated solution ϕ_{ijk}^{n+1} from Eq. (11).

To approximate the curvature on the cell-centered grid, we evaluate the discrete gradient of ϕ at the neighboring half-grid locations around the cell center (x_i, y_j, z_k) . A related discussion of isotropic finite difference stencils can be found in [Patra and Karttunen \(2006\)](#). The discrete derivative in the x -direction at the half-grid location $(x_{i+1/2}, y_{j+1/2}, z_{k+1/2})$ is defined by averaging four adjacent finite differences:

$$\begin{aligned} \nabla_x \phi_{i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2}} &= \frac{1}{4h} (\phi_{i+1, j, k} - \phi_{i, j, k} + \phi_{i+1, j+1, k} - \phi_{i, j+1, k} \\ &\quad + \phi_{i+1, j, k+1} - \phi_{i, j, k+1} + \phi_{i+1, j+1, k+1} - \phi_{i, j+1, k+1}). \end{aligned}$$

The derivatives in the y - and z -directions are defined analogously, and the same construction is applied to the other neighboring half-grid locations. Using these definitions, we introduce the discrete unit normal vector

$$\mathbf{m}_{i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2}} = \frac{\nabla_h \phi_{i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2}}}{\left| \nabla_h \phi_{i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2}} \right|},$$

where $|\nabla_h \phi| = \sqrt{(\nabla_x \phi)^2 + (\nabla_y \phi)^2 + (\nabla_z \phi)^2}$. The discrete curvature at the cell center (x_i, y_j, z_k) is computed as the discrete divergence of the unit normal vector:

$$\kappa_{ijk} = (\nabla_x m^x)_{ijk} + (\nabla_y m^y)_{ijk} + (\nabla_z m^z)_{ijk},$$

where, for example,

$$\begin{aligned} (\nabla_x m^x)_{ijk} &= \frac{1}{4h} \left(m_{i+\frac{1}{2}, j-\frac{1}{2}, k-\frac{1}{2}}^x - m_{i-\frac{1}{2}, j-\frac{1}{2}, k-\frac{1}{2}}^x + m_{i+\frac{1}{2}, j+\frac{1}{2}, k-\frac{1}{2}}^x - m_{i-\frac{1}{2}, j+\frac{1}{2}, k-\frac{1}{2}}^x \right. \\ &\quad \left. + m_{i+\frac{1}{2}, j-\frac{1}{2}, k+\frac{1}{2}}^x - m_{i-\frac{1}{2}, j-\frac{1}{2}, k+\frac{1}{2}}^x + m_{i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2}}^x - m_{i-\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2}}^x \right), \end{aligned}$$

and $(\nabla_y m^y)_{ijk}$ and $(\nabla_z m^z)_{ijk}$ are defined analogously. Therefore,

$$\kappa_{ijk} = (\nabla_h \cdot \mathbf{m})_{ijk}.$$

In practice, to avoid numerical singularities, the curvature is set to zero at grid points where $|\nabla_h \phi|$ is below a prescribed tolerance. Unlike explicit interface tracking methods, such as particle level-set methods ([Hieber & Koumoutsakos, 2005](#)), the phase-field method describes the boundary as a continuous interface layer transition. However, to strictly localize the multiplier's effect and avoid numerical singularities in the bulk phases, we use a narrow band method in practice, specifically where $|\phi| < 0.98$.

3. Computational tests

We conduct several numerical tests to verify the performance of the proposed CAC model. In particular, we focus on its ability to preserve geometric features of the interface compared with conventional CAC models. We introduce the notation $\epsilon_m = hm/[2\sqrt{2}\tanh^{-1}(0.9)]$, where m is a positive integer. This parameter corresponds to approximately m grid points across the diffuse interface; see [Yang and Kim \(2025\)](#) and the references therein for further details. Unless otherwise specified, we set $\epsilon = \epsilon_5$ throughout the simulations.

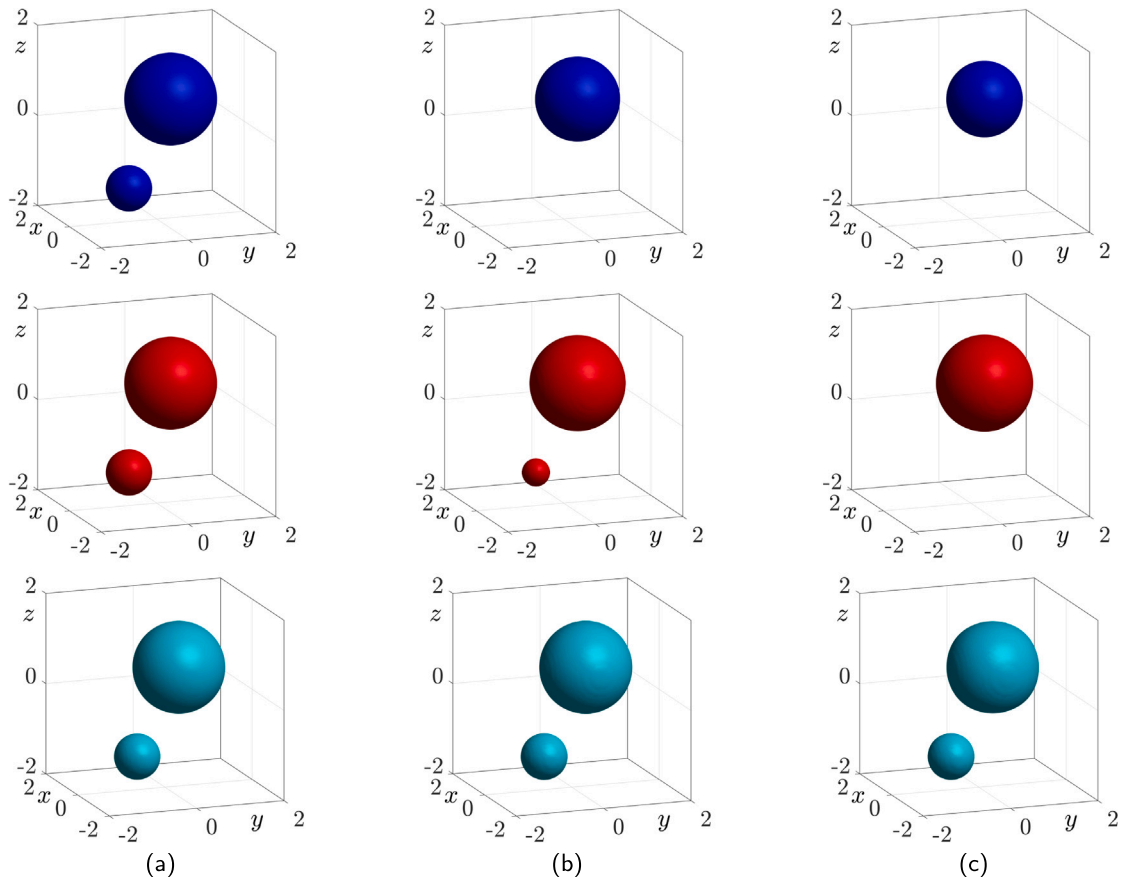


Fig. 1. Time evolution of the zero-level interfaces with different Lagrange multipliers. The rows correspond to $\gamma_1(t)$, $\gamma_2(t)\sqrt{2F(\phi)}$, and $\gamma(t)\kappa(\phi)\sqrt{2F(\phi)}$, from top to bottom. (a), (b), and (c) show the results at times $t = 0$, $20\Delta t$, and $1000\Delta t$, respectively. The phase-field interfaces are visualized using different colors (blue, red, and cyan) to distinguish the solutions corresponding to different conservation formulations.

3.1. Geometric feature preservation

We study the behavior of the proposed CAC model through numerical tests. We compare the results with two widely used CAC models. The computational domain is given by $\Omega = (-2, 2) \times (-2, 2) \times (-2, 2)$. We use two spheres as the initial condition:

$$\phi(x, y, z, 0) = 1 + \tanh\left(\frac{0.5 - \sqrt{(x+1)^2 + (y+1)^2 + (z+1)^2}}{\sqrt{2}\epsilon}\right) + \tanh\left(\frac{1 - \sqrt{(x-0.5)^2 + (y-0.5)^2 + (z-0.5)^2}}{\sqrt{2}\epsilon}\right).$$

The spatial mesh size is $h = 0.0625$, and the time step is set as $\Delta t = h^2$. Fig. 1 shows the computational results for different Lagrange multipliers. The top and middle rows show the results for $\gamma_1(t)$ and $\gamma_2(t)\sqrt{2F(\phi)}$, respectively. In both cases, the small sphere gets smaller, and the large sphere gets larger. At the end, the small sphere disappears, and only one sphere is left. These results show that the standard CAC models do not keep the initial shapes. The bottom row shows the result for the curvature-dependent Lagrange multiplier, $\gamma(t)\kappa(\phi)\sqrt{2F(\phi)}$. In this case, both spheres keep their shapes. This numerical result shows that the proposed model keeps the initial shapes and prevents the small sphere from disappearing. Fig. 1(c) shows the evolution at $t = 1000\Delta t$ (i.e., $t = 3.90625$). As observed, the proposed model successfully preserves the prescribed shape, even under long-time simulation.

Next, we consider a more complex initial interface. We examine the ability of the proposed model to preserve geometric features. We define the initial condition in $\Omega = (-2, 2) \times (-2, 2) \times (-2, 2)$ as

$$\phi(x, y, z, 0) = \tanh\left(\frac{R(\theta, \psi) - r}{\sqrt{2}\epsilon}\right), \quad (14)$$

where $r = \sqrt{x^2 + y^2 + z^2}$, $\theta = \cos^{-1}(z/r)$, $\psi = \arctan(y/x)$. $R(\theta, \psi) = 1.2 + 0.5 \sin(4\theta) \sin(5\psi)$ is the radius function. This initial condition represents a perturbed sphere with non-uniform curvature. The mesh size is $h = 4/64$, and the time step is $\Delta t = 0.1h^2$. The equilibrium

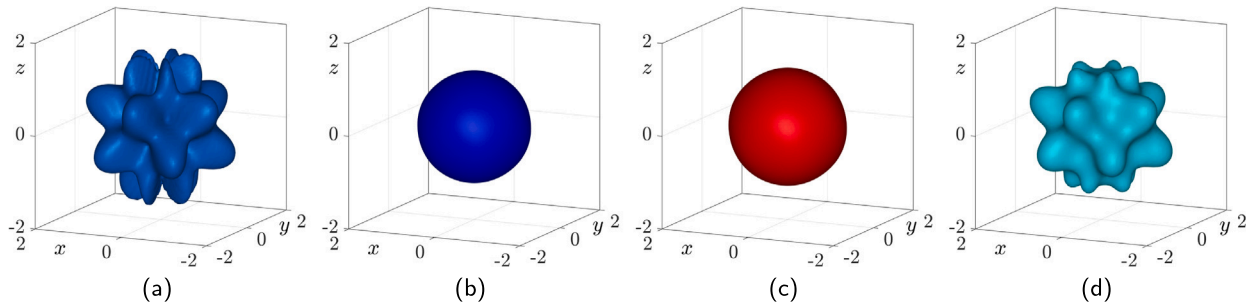


Fig. 2. (a) is the initial condition. (b), (c), and (d) are the numerical equilibrium results for $\gamma_1(t)$, $\gamma_2(t)\sqrt{2F(\phi)}$, and $\gamma(t)\kappa(\phi)\sqrt{2F(\phi)}$, respectively. The zero-level isosurfaces are shown in blue, red, and cyan.

state is defined by $\|\phi^{n+1} - \phi^n\|_2 < \text{tol}$, $\text{tol} = 10^{-4}$. Fig. 2 shows the final interfaces with different Lagrange multipliers. In the previous models, the interface becomes a smooth sphere, and the initial small features disappear. This numerical result means that curvature makes the interface smooth and removes small details. In contrast, the proposed equation keeps the shape of the interface. The uneven surface features still appear at the final state. This computational result means that the proposed model reduces excessive smoothing and keeps geometric details (see Fig. 3).

Now, we consider the initial condition defined in Eq. (14) with finer mesh size $h = 4/128$, smaller time step $\Delta t = 0.05h^2$, and thinner interfacial parameter $\epsilon = \epsilon_3$. It can be seen that the proposed model can preserve the features with better accuracy.

We further consider an initial configuration consisting of a sphere and a cube in $\Omega = (-0.5, 0.5) \times (-0.5, 0.5) \times (-1, 1)$. The initial condition is defined as

$$\phi(x, y, z, 0) = 1 + \tanh\left(\frac{0.15 - \sqrt{x^2 + y^2 + (z - 0.35)^2}}{\sqrt{2}\epsilon}\right) + \tanh\left(\frac{-\max(|x| - 0.48, |y| - 0.48, |z + 0.75| - 0.2)}{\sqrt{2}\epsilon}\right).$$

A uniform mesh with $h = 1/64$ is used, and the time step is taken as $\Delta t = 0.1h^2$. Fig. 4 displays the temporal evolution of the interfaces. For the conventional models, the sphere shrinks and eventually disappears, while the cube expands. The computational results show that the large shape gets larger, and the small shape gets smaller because of curvature. The proposed model keeps both the sphere and the cube. Both shapes stay the same during the simulation. These results show that the proposed model keeps both shapes and does not let the small structure disappear. Moreover, if gravity is added, the sphere above the cube falls. The proposed model gives a more accurate result because it keeps the sphere from becoming smaller or disappearing during its motion. Therefore, it captures the real physical motion more accurately.

3.2. Interface evolution under a given velocity field

Next, we test the proposed model with a given velocity field. Accurate and conservative treatment of advection is important for interface evolution under incompressible flow (LeVeque, 1996). This test shows whether the method stays stable and keeps the interface shape under advection. The same benchmark was previously considered by Enright et al. (2002) using a level-set method. The governing equation is given by

$$\partial_t \phi + \nabla \cdot [\phi \mathbf{u}(x, y, z)] = \frac{1}{Pe} \left[-\frac{F'(\phi)}{\epsilon^2} + \Delta \phi + \gamma(t)\kappa(\phi)\sqrt{2F(\phi)} \right], \quad (15)$$

where Pe is the Péclet number. In this test, we set $Pe = 100$. The advection term in Eq. (15) is discretized using a finite difference method with central differences in space. The velocity field $\mathbf{u}(x, y, z) = (u(x, y, z), v(x, y, z), w(x, y, z))$ is defined as

$$\begin{aligned} u(x, y, z) &= 2 \sin^2(\pi x) \sin(2\pi y) \sin(2\pi z), \\ v(x, y, z) &= -\sin(2\pi x) \sin^2(\pi y) \sin(2\pi z), \\ w(x, y, z) &= -\sin(2\pi x) \sin(2\pi y) \sin^2(\pi z). \end{aligned}$$

This velocity field (LeVeque, 1996) creates a swirling motion. This motion deforms and transports the interface. The initial condition is defined in the domain $\Omega = (0, 1) \times (0, 1) \times (0, 1)$ as

$$\phi(x, y, z, 0) = \tanh\left(\frac{0.15 - \sqrt{(x - 0.35)^2 + (y - 0.35)^2 + (z - 0.35)^2}}{\sqrt{2}\epsilon}\right).$$

The numerical parameters are given by $T = 0.8$, $h = 0.01$, and $\Delta t = h^2$. Fig. 5 shows how the droplet changes over time. The velocity field stretches and turns the interface. Over time, the droplet changes its shape a lot, but the interface stays smooth. This numerical

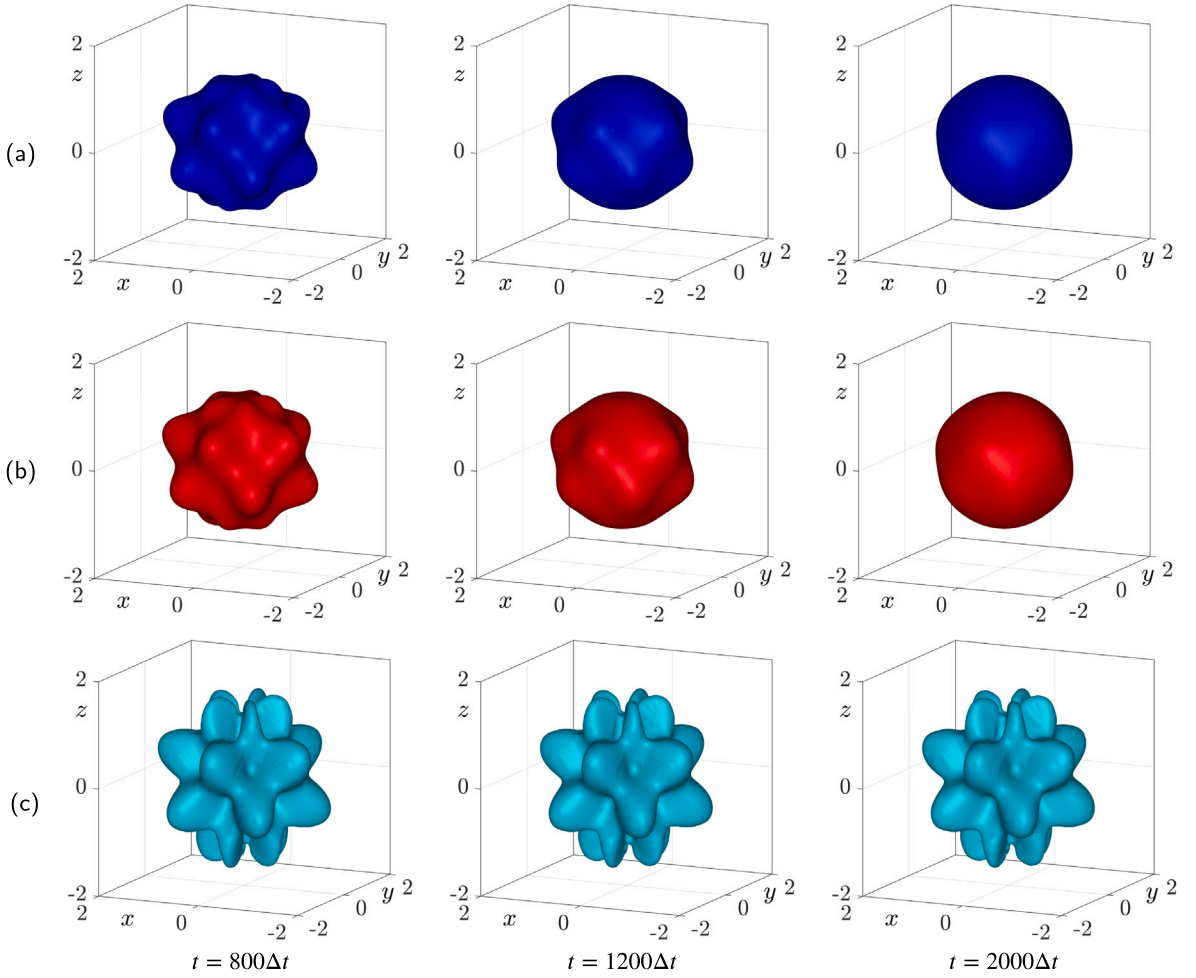


Fig. 3. The rows correspond to (a) $\gamma_1(t)$, (b) $\gamma_2(t)\sqrt{2F(\phi)}$, and (c) $\gamma(t)\kappa(\phi)\sqrt{2F(\phi)}$. The columns correspond to the results at times $t = 800\Delta t$, $1200\Delta t$, and $2000\Delta t$, respectively. The zero-level phase-field interfaces are visualized using different colors (blue, red, and cyan) to distinguish the solutions corresponding to different conservation formulations.

result shows that the proposed 3D model stays stable under motion. The interface does not break or show numerical noise. The proposed model also keeps the shape without artificial changes. This shows that the proposed model can handle both curvature effects and transport in a stable way.

3.3. Comparison with the CH model

Now, we compare the equilibrium performance of the proposed CAC model with the CH model proposed in Lee et al. (2020) in three dimensions. In Lee et al. (2020), the authors documented that the 3D CH equation minimizes the total bulk and interfacial energy by allowing the interface to shrink, which requires a large number of grid points across the radius to preserve a droplet shape at equilibrium. To demonstrate that the proposed model can preserve spherical structures under a much smaller initial radius condition where the CH model suffers from severe size regression, we perform a numerical test in a cubic domain $\Omega = (0, 1) \times (0, 1) \times (0, 1)$ with a mesh size of $h = 1/64$. The initial condition is given by a single spherical droplet:

$$\phi(x, y, z, 0) = \tanh\left(\frac{R_0 - \sqrt{(x - 0.5)^2 + (y - 0.5)^2 + (z - 0.5)^2}}{\sqrt{2}\epsilon}\right),$$

where the initial radius is chosen as $R_0 = 5h$. The interface parameter is set to $\epsilon = \epsilon_4$, and the time step size is $\Delta t = 0.1h^2$. In this test, the CH model requires an initial radius of at least 19 h to maintain a droplet solution at equilibrium. In contrast, we test the proposed CAC model with an initial radius of 5 h. We stop the simulation when $\|\phi^{n+1} - \phi^n\|_2 < 10^{-10}$. This means that the solution has reached numerical equilibrium.

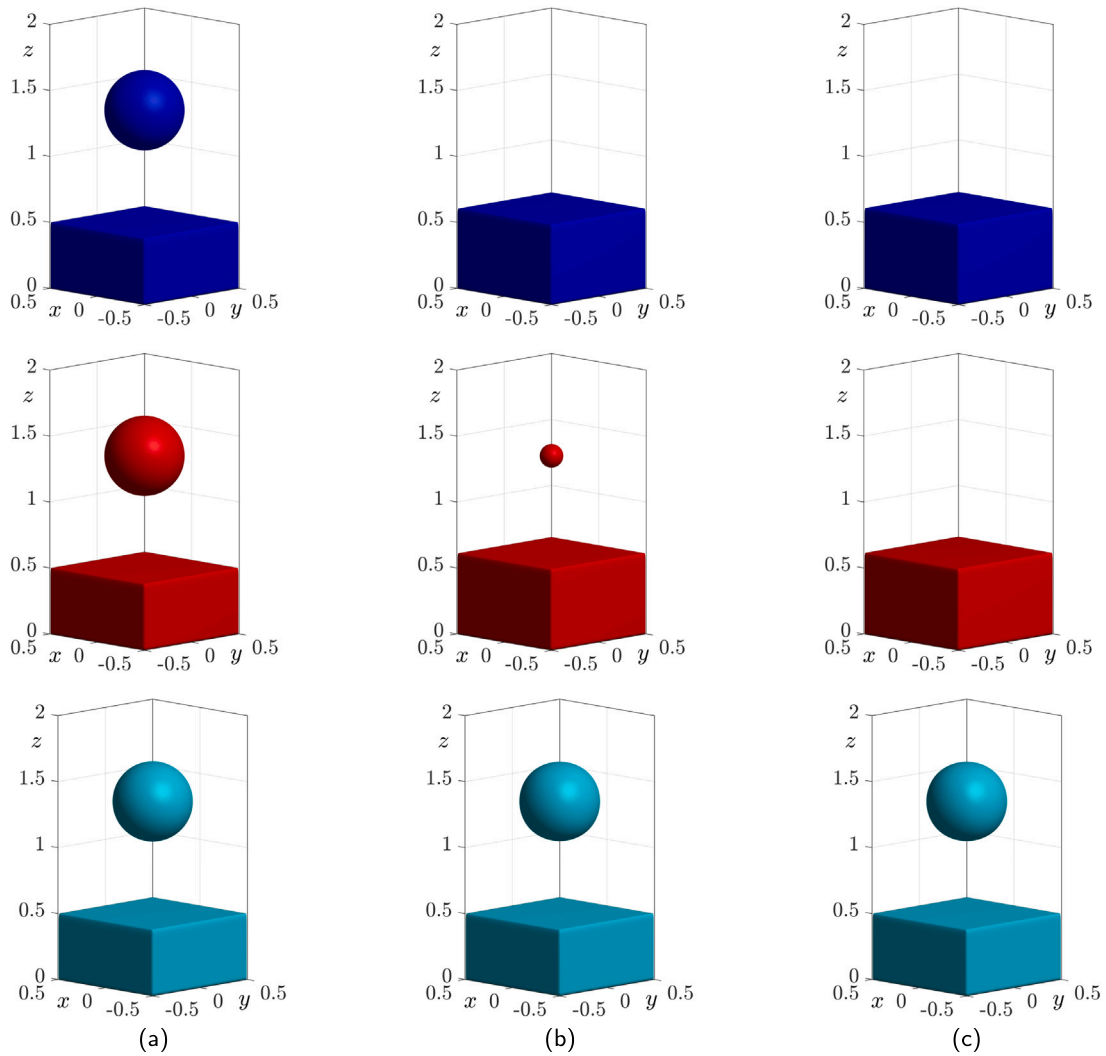


Fig. 4. Evolution of the zero-level interfaces for three Lagrange multipliers. The results are organized in three rows. The top row uses $\gamma_1(t)$, the middle row uses $\gamma_2(t)\sqrt{2F(\phi)}$, and the bottom row uses $\gamma(t)\kappa(\phi)\sqrt{2F(\phi)}$. Snapshots are shown at (a) $t = 0$, (b) $t = 1360\Delta t$, and (c) $t = 1440\Delta t$.

Fig. 6 shows the numerical equilibrium profiles obtained from both models. The equilibrium radius for the CH model is approximately $r_{CH} = 0.21728$, and the equilibrium radius for the proposed CAC model is $r_{CAC} = 0.07676$. The ratio of the equilibrium radii is $r_{CH}/r_{CAC} \approx 2.83$. This ratio becomes smaller than the initial radius ratio ($19h/5h = 3.8$). This is because the CH model loses a large amount of the volume inside the zero-level isosurface, while the proposed CAC model preserves almost all of its initial volume at the steady state. This quantitative comparison confirms that the proposed model provides a more robust and grid-efficient method for 3D simulations containing small-scale geometric features.

3.4. Practical applicability to droplet transport

To illustrate the potential applicability of the proposed model, we consider the transport of 3D droplets with different sizes. Preservation of small droplets is important in microfluidic systems, where dispersed droplets are transported by a continuous fluid phase. For example, Dewandre et al. (2020) experimentally studied water-droplet generation in a continuous light mineral oil phase. In such systems, artificial curvature-driven shrinkage in a numerical model may lead to inaccurate predictions of droplet size or even disappearance of small droplets.

Motivated by this application, we examine whether the proposed model can transport small droplets without significant changes in their volume and geometric features. We use a prescribed constant velocity field to provide a simple and controlled numerical setting. This test is intended to demonstrate the potential usefulness of the proposed mathematical model for droplet transport rather than to reproduce or validate a specific physical experiment. A complete physical description would require coupling the phase-field model with the governing fluid equations.

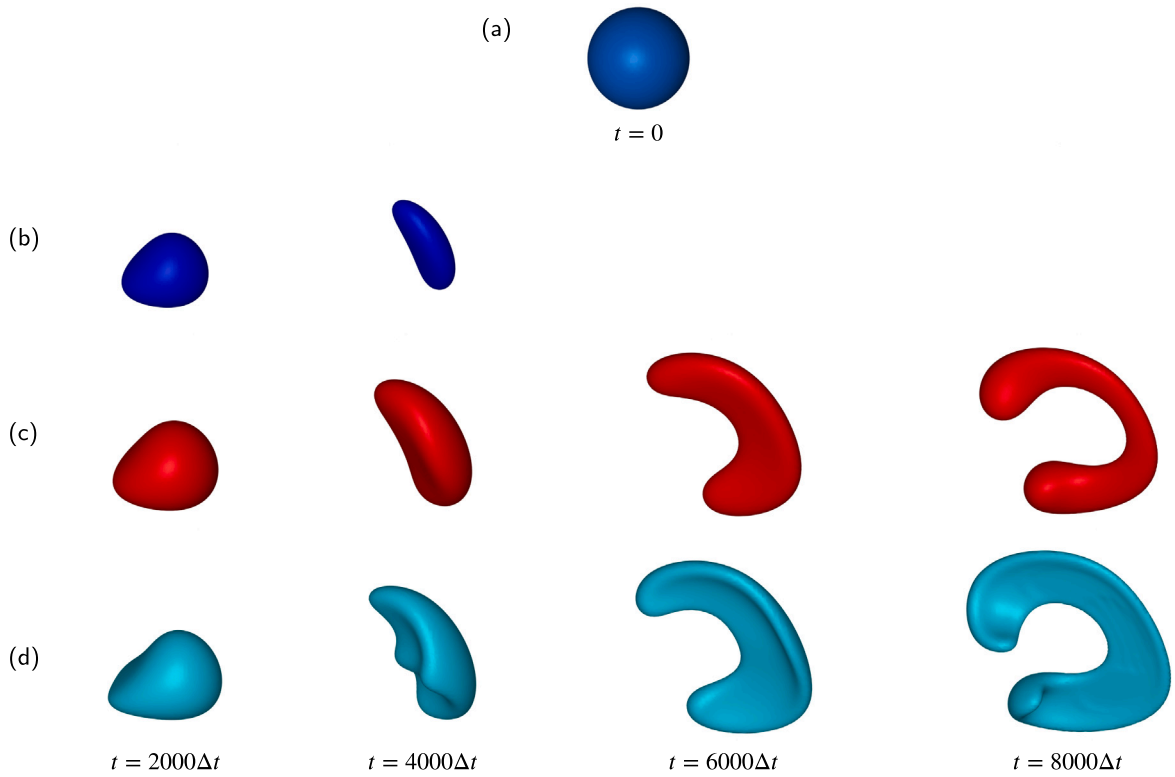


Fig. 5. Evolution of the zero-level interfaces for different Lagrange multipliers. The rows from top to bottom correspond to (b) $\gamma(t)$, (c) $\gamma(t)\sqrt{2F(\phi)}$, and (d) $\gamma(t)\kappa(\phi)\sqrt{2F(\phi)}$. (a) shows a snapshot at time $t = 0$. From the first column to the last column of (b), (c), and (d), temporal evolutions at times $t = 2000\Delta t$, $t = 4000\Delta t$, $t = 6000\Delta t$, and $t = 8000\Delta t$ are presented. The phase-field interfaces are visualized using different colors (blue, red, and cyan) to distinguish the solutions corresponding to different conservation formulations.

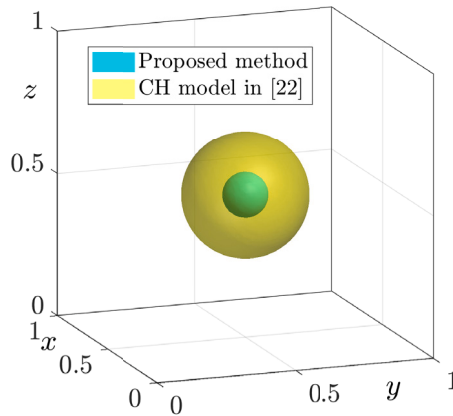


Fig. 6. Comparison of the numerical equilibrium states ($\phi = 0$) between the CH model in Lee et al. (2020) (outer yellow isosurface) and the proposed CAC model (inner cyan isosurface).

We consider the computational domain $\Omega = (0, 6) \times (-0.4, 0.4) \times (-0.4, 0.4)$. A uniform mesh with $h = 0.02$ is used. The time step is $\Delta t = 0.1h^2$, the final time is $T = 1.2$, and the Peclet number is $Pe = 100$. We set the interfacial parameter to $\epsilon = \epsilon_8$. The initial condition consists of three spherical droplets with different radii. Their radii are $R_1 = 0.25$, $R_2 = 0.2$, and $R_3 = 0.15$, respectively. The initial condition is defined by

$$\phi(x, y, z, 0) = \tanh\left(\frac{R_1 - \sqrt{(x-0.5)^2 + y^2 + z^2}}{\sqrt{2}\epsilon}\right) + \tanh\left(\frac{R_2 - \sqrt{(x-1.5)^2 + y^2 + z^2}}{\sqrt{2}\epsilon}\right)$$

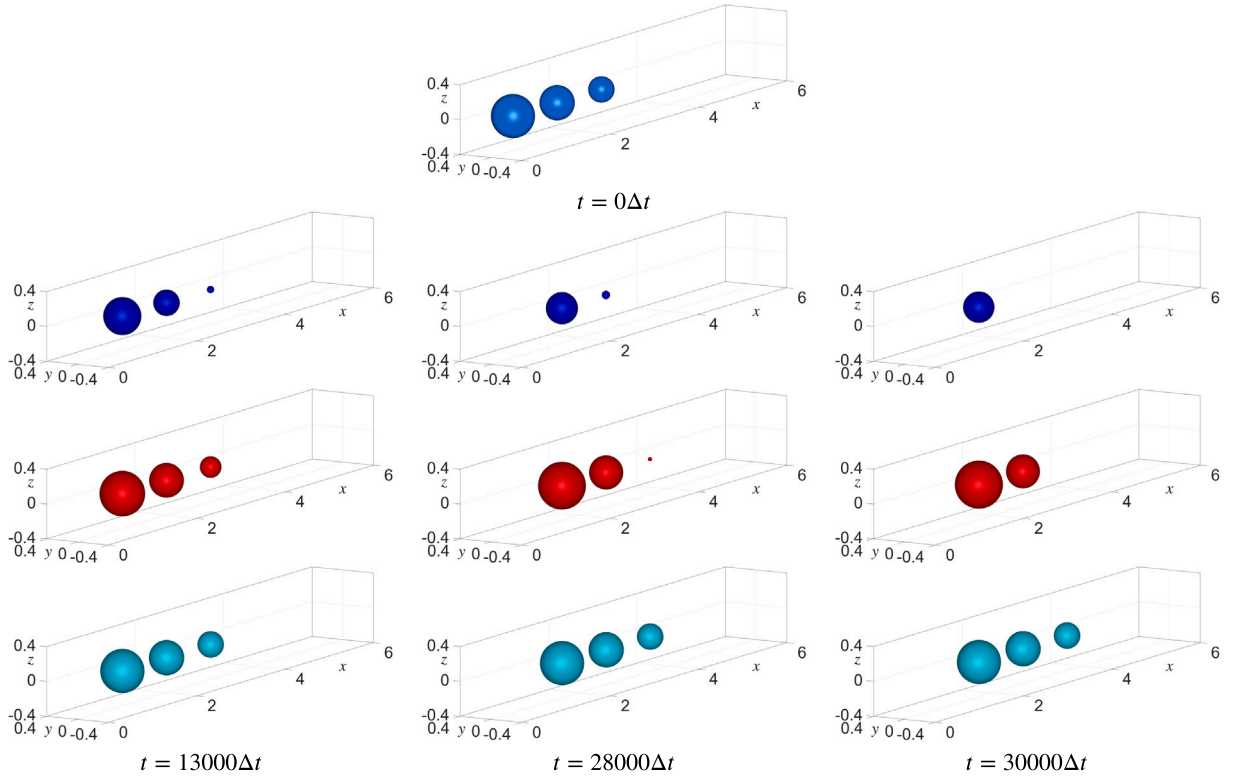


Fig. 7. Evolution of the zero-level interfaces under the prescribed uniform velocity field. From top to bottom, the rows correspond to the CAC models with $\gamma_1(t)$, $\gamma_2(t)\sqrt{2F(\phi)}$, and the proposed curvature-dependent term $\gamma(t)\kappa(\phi)\sqrt{2F(\phi)}$, respectively. The columns show the numerical solutions at the times indicated below each panel. The initial droplet radii are $R_1 = 0.25$, $R_2 = 0.20$, and $R_3 = 0.15$.

$$+ \tanh\left(\frac{R_3 - \sqrt{(x - 2.5)^2 + y^2 + z^2}}{\sqrt{2}\epsilon}\right) + 2.$$

We prescribe the velocity field $\mathbf{u}(x, y, z) = (1, 0, 0)$. Thus, the flow transports all droplets in the positive x -direction at the same speed. The computational domain is sufficiently long so that all droplets remain separated from the boundaries during the simulation. This experiment tests droplets of three different sizes under the same transport condition. In particular, the smallest droplet provides a sensitive test of artificial curvature-driven shrinkage.

Fig. 7 shows the evolution of the zero-level interfaces under the prescribed constant flow. All three droplets move in the positive x -direction. However, their interface behaviors differ during transport. In the conventional CAC models, the smaller droplets gradually shrink, whereas the larger droplet grows. This behavior occurs because the conventional Lagrange multipliers preserve only the total mass and do not prevent curvature-driven mass transfer between droplets of different sizes. Consequently, the smallest droplet may disappear even though the total mass remains constant.

In contrast, the proposed model preserves their spherical shapes and prevents the smaller droplets from disappearing during transport. These results indicate that the proposed model can maintain individual droplet structures in an advection-dominated setting. This property is relevant to oil-based microfluidic systems, where inaccurate curvature effects may change the predicted droplet-size distribution.

4. Conclusions

In this study, we proposed a 3D CAC model with a curvature-dependent Lagrange multiplier. The proposed model conserved the total mass and reduced unwanted curvature effects. As a result, it preserved small structures and complex interface shapes better than the standard CAC models. We also developed a simple numerical method based on OSM, DCT, an exact solution for the reaction term, and FDM for curvature calculation. The numerical results showed that the proposed model preserved interface shapes, remained stable under a given velocity field, and outperformed the CH model in preserving small droplets. These computational results show that the proposed model is a simple and effective method for 3D simulations that require both mass conservation and shape preservation. The proposed formulation is a mathematically motivated modification designed to suppress curvature-driven interface motion, and it is not derived from an established physical or thermodynamic principle. Therefore, further theoretical studies are needed to establish its energetic structure and to clarify the relationship between the model parameters and physical surface

tension. Future work will include the development of a maximum-principle-preserving numerical scheme and applications to fluid flow and more general multiphase problems.

CRediT authorship contribution statement

Soobin Kwak: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Conceptualization. **Xinpei Wu:** Writing – review & editing, Writing – original draft, Visualization, Software. **Junseok Kim:** Writing – review & editing, Writing – original draft, Validation, Supervision, Project administration, Methodology, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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