

## SPECIAL ISSUE PAPER

# A Versatile Energy-Based SPH Surface Tension With Spatial Gradients

Qianwei Wang<sup>1</sup>  | Yanrui Xu<sup>1</sup>  | Xiangyu Sheng<sup>1</sup> | Chao Yao<sup>2</sup>  | Yu Guo<sup>2,3</sup> | Jian Chang<sup>4</sup> | Jianjun Zhang<sup>3</sup> | Xiaokun Wang<sup>1,3</sup> 

<sup>1</sup>School of Intelligence Science and Technology, University of Science and Technology Beijing, Beijing, China | <sup>2</sup>School of Computer and Communication Engineering, University of Science and Technology Beijing, Beijing, China | <sup>3</sup>Shunde Innovation School, University of Science and Technology Beijing, China | <sup>4</sup>National Centre for Computer Animation, Bournemouth University, Poole, UK

**Correspondence:** Chao Yao ([yaochao@ustb.edu.cn](mailto:yaochao@ustb.edu.cn)) | Xiaokun Wang ([wangxiaokun@ustb.edu.cn](mailto:wangxiaokun@ustb.edu.cn))

**Received:** 30 April 2025 | **Accepted:** 14 May 2025

**Funding:** This work was supported by Basic and Applied Basic Research Foundation of Guangdong Province (Grant No. 2023A1515030177), National Natural Science Foundation of China (Grant Nos. 62376025 and 62332017), Key Research and Development Program of Hainan Province (ZDYF2024GXJS032) and National High Level Hospital Clinical Research Funding (2022-PUMCH-D-004).

**Keywords:** fluid simulation | interface energy | Marangoni effect | surface tension | wetting

## ABSTRACT

We propose a novel simulation method for surface tension effects based on the Smoothed Particle Hydrodynamics framework, capturing versatile tension effects using a unified interface energy description. Guided by the principle of energy minimization, we compute the interface energy from multiple interfaces solely using the original kernel function estimation, which eliminates the dependence on second-order derivative discretization. Subsequently, we incorporate an inertia term into the energy function to strike a balance between tension effects and other forces. To simulate tension, we propose an energy diffusion-based method for minimizing the objective energy function. The particles at the interface are iteratively shifted from high-energy regions to low-energy regions through several iterations, thereby achieving global interface energy minimization. Furthermore, our approach incorporates surface tension parameters as variable quantities within the energy framework, enabling automatic resolution of tension spatial gradients without requiring explicit computation of interfacial gradients. Experimental results demonstrate that our method effectively captures the wetting, capillary, and Marangoni effects, showcasing significant improvements in both the accuracy and stability of tension simulation.

## 1 | Introduction

Surface tension exerts substantial influence on various fluid phenomena in nature, particularly in the formation of liquid droplets [1, 2], thin-film bubbles [3–5], and capillary phenomenon [6, 7]. The interfacial dynamics between fluids and solid surfaces also give rise to complex behaviors, including hydrophilic and hydrophobic effects [6, 8]. These complex physical processes have attracted significant attention in the field of

computer graphics [9], prompting simulation studies aimed at achieving increasingly refined and realistic visual effects.

At the microscale, surface tension fundamentally arises from asymmetric molecular attraction forces at fluid interfaces. This imbalance induces tangential stress fields that minimize interfacial area through contractile forces. However, resolving such intermolecular potential gradients requires molecular-scale discretization, rendering direct molecular dynamics simulations

**Abbreviations:** CSF, continuum surface force; MPM, material point method; SPH, smoothed particle hydrodynamics.

computationally prohibitive. To circumvent this limitation at continuum scales, effective modeling has been achieved in Smoothed Particle Hydrodynamics (SPH). The pairwise force model was developed to simulate surface tension following the microscopic principle [1, 2, 10, 11]. Nevertheless, compared with true molecular interactions, these methods require carefully tuned interaction functions to artificially enhance short-range cohesion and suppress repulsive forces, thus reducing particle clustering.

To enhance simulation fidelity, the continuum surface force (CSF) model employs macroscopic principles of surface energy minimization, calculating surface tension through local curvature estimation to reduce interfacial area. However, the CSF model faces challenges in accurately capturing curvature near the free surface due to insufficient particle sampling, which undermines both computational efficiency and numerical stability. Furthermore, the CSF model exhibits intrinsic limitations in capturing interface migration phenomena driven by surface tension spatial gradients, specifically the Marangoni effect. Tong and Browne [12] introduced an interfacial gradient term  $\nabla_s$  in the CSF formulation to expand the model. However, this approach lacks thermodynamic consistency, and the numerical computation of the interfacial gradient also introduces non-negligible errors.

To overcome these limitations, we introduce a novel tension model driven by interface energy, which formulates versatile interfacial effects within a unified energy framework. Our model addresses energy contributions at liquid–gas, liquid–liquid, liquid–solid, and gas–solid interfaces, obtaining the interface energy function for both fluid and solid particles. To eliminate dependence on second-order derivatives, we employ an original SPH kernel estimation formulation for interfacial area calculation, which is proposed by Probst and Teschner [7]. We combine it with solid volume resampling to enhance area estimation accuracy in solid-involved interfaces.

Subsequently, we extended the energy function by introducing an inertia term [13] and implement an energy diffusion-based method to drive particles transition from high-energy regions to low-energy regions, achieving minimization of the interface area, which is consistent with the effect of tension. The energy minimization of multiple interfaces enables the unified treatment of phenomena such as high surface tension coefficients, wettability, and capillary forces within a single framework.

Furthermore, we incorporate spatially varying tension coefficients into the derivation, allowing particles at the interface to experience traction from neighboring interfacial particles with higher tension coefficients. This allows spontaneous initiation of the Marangoni effect without requiring explicit computation of complex interfacial spatial gradients.

## 2 | Related Work

### 2.1 | Pairwise Force Models

Surface tension arises from unbalanced molecular interactions at the microscopic level. Several studies approximate these

interactions macroscopically by introducing suitable attractive and repulsive forces between adjacent particles [2, 9, 14, 15]. Most of these methodologies suffer from particle clustering problems, resulting in simulation artifacts and numerical instabilities. Yang et al. [6] developed a cosine-based interaction force function to mitigate particle clustering by generating repulsive effects when particles are close to each other. Jeske et al. [11] developed an implicit pairwise tension model, achieving stable simulations of cohesion and adhesion.

### 2.2 | Continuum Surface Force Models

The CSF model operates through macroscopic tension effects, applying curvature-dependent volumetric forces to fluids to facilitate surface area minimization. Brackbill et al. [16] constructed smooth transition interfaces using color field functions in particle methods to represent surfaces, facilitating precise normal vector estimation at material interfaces, which subsequently enables curvature computation through gradient operations. Due to satisfactory performance and accuracy, the CSF model has been widely implemented in SPH-based methodologies. However, the estimation of normals can easily generate noise inside the fluid, and the presence of second-order derivatives makes the calculation highly sensitive to particle disorder [1, 17, 18]. To improve numerical robustness, He et al. [19] developed an air phase sampling approximation to address insufficient particle sampling on free surfaces. Adami et al. [18] proposed a reproducing divergence approximation to compute curvature and alleviate errors caused by second-order estimation. Expanding the CSF model, Tong and Browne [12] incorporated thermal capillary into the CSF model and introduced an interfacial gradient term to handle variable tension, achieving simulation of the Marangoni effect.

### 2.3 | Hybrid Models

Some studies attempted to combine the above two methods to simultaneously obtain both advantages [1, 9]. In addition, various numerical methods have been developed to simulate surface tension. Da et al. [20] proposed a mesh-based surface-only fluid simulation framework capable of resolving microscale surface tension phenomena with high fidelity. Wang et al. [3] utilized co-dimensional particles to model fluid sheets and filaments. Xing et al. [21] developed a method to simulate surface tension effects by constructing local one-ring meshes around surface particles and minimizing their areas. Energy-based methodologies have garnered increasing attention in recent years. Hyde et al. [22] developed a variational formulation for Material Point Method (MPM), subsequently extended by Chen et al. [23] to incorporate thermal phase transitions. Compared with other methods, the energy-based formulation enables the unified simulation of surface tension alongside other physical phenomena, which can be incorporated by an energy framework [7, 24]. Probst and Teschner [7] proposed a novel method for computing surface energy within the SPH framework and simulated physically consistent surface tension effects using an implicit formulation.

## 3 | SPH Fundamentals

Since our approach adopts a particle-based description, our methodology is fundamentally grounded in the SPH framework.



In SPH, the fluid is discretized into a series of particles that carry physical properties. The physical quantity  $A_i$  of a certain fluid particle  $i$  at position  $\mathbf{x}_i$  is approximated through interpolation of the corresponding physical quantities of other particles within a certain spatial domain,

$$A_i = \sum_j A_j V_j W(\mathbf{x}_i - \mathbf{x}_j, h) \quad (1)$$

where the subscript  $j$  denotes a neighboring particle,  $V$  denotes volume,  $\mathbf{x}$  denotes position. The kernel function  $W$  is a Gaussian-like function, chosen to be a cubic spline as suggested by Monaghan [25], and  $h$  denotes the support radius of  $W$ , which is typically double the value of particle sampling distance  $d_0$ . For the sake of brevity and readability,  $W(\mathbf{x}_i - \mathbf{x}_j, h)$  is replaced by  $W_{ij}$  in the following text.

For solids, we also employ a unified particle representation. Taking into account uneven sampling, we perform volumetric sampling of solid particles referencing the resampling method proposed by Akinici et al. [1]. The volume of a solid particle  $b_i$  can be approximated as:

$$V_{b_i} = \frac{1}{\sum_{b_j} W_{b_i b_j}} \quad (2)$$

where  $b_j$  is a solid neighbor.

The volume of fluid particle  $i$  can be calculated as:

$$V_i = \frac{V_0}{\sum_j V_0 W_{ij} + \sum_b V_b W_{ib}} \quad (3)$$

where  $j$  is a fluid neighbor,  $b$  is a solid neighbor, and  $V_0$  is the rest volume of a fluid particle, as we assume that all fluid particles have the same rest volume.

## 4 | Method

In this section, we propose a tension computation framework based on energy minimization principles, which comprises an interface energy estimation method and an energy diffusion-driven tension mechanism.

### 4.1 | Interface Energy Estimation

The interface energy  $E_{st}$  associated with the formation of the interface is proportional to the interface area  $A_{st}$ , which can be calculated as:

$$E_{st} = \sigma A_{st} \quad (4)$$

where  $\sigma$  is the respective energy density or also called the tension coefficient.

For the entire system, the interface energy not only exists on the surface of the liquid but is also stored on the surface of the solid. To capture the behavior of interfacial interaction between the liquid and the solid, this part is indispensable. Therefore, the total interface energy should be calculated as follows:

$$E_{st}^{\text{total}} = E_{st}^L + E_{st}^S \quad (5)$$

where  $E_{st}^L$  denotes the interface energy on liquid surface,  $E_{st}^S$  on solid surface. In most works, to simulate the cohesive effects between liquids and the adhesive effects between liquids and solids, the liquid–gas and solid–liquid interfaces are typically considered, while the solid–gas interface is typically neglected [23]. However, in order to achieve a unified description of all interfaces and enable flexible parameter tuning, the solid–gas interface must be explicitly incorporated. Furthermore, in multiphase flow scenarios, interfaces also exist between distinct liquid phases, necessitating the contributions of the liquid–liquid interface. At this stage, the total interface energy that encompasses all interfaces can be expressed as:

$$E_{st}^L = \sigma^{LG} A_{st}^{LG} + \sigma^{LL^*} A_{st}^{LL^*} + \sigma^{LS} A_{st}^{LS} \quad (6a)$$

$$E_{st}^S = \sigma^{SG} A_{st}^{SG} + \sigma^{SL} A_{st}^{SL} \quad (6b)$$

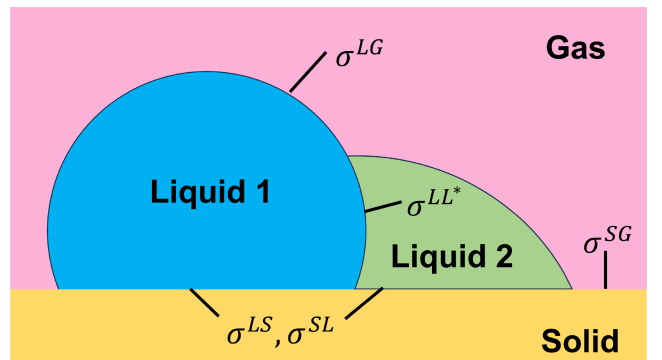
where  $LG$  denotes the liquid–gas interface,  $LL^*$  denotes the interface between  $L$  and another liquid phase  $L^*$  and  $LG$  denotes the liquid–solid interface. The spatial schematic diagram of multiphase interfaces is shown in Figure 1.

It is evident that the estimation of the interface area  $A$  is a crucial factor. In most SPH-based methods, the gradient of the color function is typically used to calculate the interface area [19, 26]. However, this approach introduces second-order derivatives when deriving forces, which exhibit high sensitivity to the particle distribution and severely affect the numerical accuracy. Probst and Teschner [7] proposed a method for computing the interface area based on the estimation of the SPH basic kernel, which is notably simpler and free of first-order derivatives. The main idea is to approximate the volume fraction of particles from different phases within the neighborhood as the surface area fraction of the corresponding interface around the particle. Firstly, we estimate the interface contribution  $C$  from all different phases within the support domain of particle  $i$ , which can be calculated as:

$$C_i^{LL^*} = \sum_{j \in L^*} V_j^0 W_{ij} \quad (7a)$$

$$C_i^{LS} = \sum_b V_b W_{ib} \quad (7b)$$

$$C_i^{LG} = 1 - \sum_j V_j^0 W_{ij} - \sum_b V_b W_{ib} \quad (7c)$$



**FIGURE 1** | Interface diagram in multiphase environment. As long as different phases of matter come into contact, an interface will exist and store energy.

The SPH method rarely directly models gas particles. However, based on the normalization property of the kernel function, the contribution of the gas phase within the support domain can be calculated by subtracting the contributions of all neighboring particles from 1, as shown in Equation (7c). Taking into account non-homogeneous sampling of solids, we replaced the solid rest volume  $V_b^0$  in [7] with the resampled volume  $V_b$  calculated by Equation (2) to generate a more precise estimate. Similarly, the interface contributions on a solid particle can be calculated as follows:

$$C_{b_i}^{SL} = \sum_{f_j} V_{f_j}^0 W_{b_i f_j} \quad (8a)$$

$$C_{b_i}^{SG} = 1 - \sum_{b_j} V_{b_j} W_{b_i b_j} - \sum_{f_j} V_{f_j} W_{b_i f_j} \quad (8b)$$

where  $f_j$  denotes a fluid neighbor and  $b_j$  denotes a solid neighbor.

To avoid discontinuity of gradients and negative value, the contribution  $C$  is typically transformed into a continuous and non-negative function  $\tilde{C}_i$ , which can be expressed as:

$$\tilde{C}_i = \max(-\xi + \sqrt{C_i^2 + \xi^2}, 0) \quad (9)$$

where  $\xi$  is a coefficient that determines the threshold for the original  $C_i$ . In our experimental practice, we set the parameter  $\xi$  to 0.1. This modification significantly improves the precision of interfacial region identification while effectively minimizing the misclassification of bulk-phase particles as interface particles.

Similar to volume discretization, each particle can be conceptualized as possessing a finite surface area, which is partitioned by interfacial regions with surrounding materials. Therefore, the volumetric weightings of different phases in the particle support domain equivalently represent their interface area weightings. With the contribution function of a specific interface, the respective interface area can be computed as the product of the function and the particle's rest surface area:

$$A = A_0 \tilde{C} \quad (10)$$

where  $A_0$  denotes the rest surface area of a particle, which is determined as  $\frac{\pi}{4} d_0^2$ . With the quantification of all interface areas, the aggregate interface energy of the system can be computed via integration over all defined interface energy density functions.

## 4.2 | Energy Diffusion-Driven Tension

The target is to minimize the energy function while achieving the tension effects and preserving the dynamic behavior. We adopt an energy diffusion-based strategy that iteratively displaces particles from regions of high-energy density to regions of low-energy density.

Inspired by the projective dynamics framework [13], our free energy minimization scheme explicitly incorporates a regularization term, which serves a role similar to that of the momentum potential. Consequently, the objective energy function to be minimized is formulated as:

$$\epsilon_i = \frac{1}{2} \frac{\|\mathbf{x}_i - \mathbf{x}_i^*\|^2}{d_0^2} + E_i \quad (11)$$

where  $d_0$  is the particle sampling distance,  $\mathbf{x}_i^*$  is the original position in current time step,  $E_i$  is the total interface energy on particle  $i$ . The first term on the right-hand side of Equation (11) requires us to achieve a balance between inertia and tension, thereby preventing instability induced by excessive particle displacement from their original positions.

Particle shifting is a commonly used particle regularization method in SPH [27]. It follows Fick's law of diffusion to shift particles from high-concentration regions to low-concentration regions, preventing excessive particle clustering. He et al. [28] applied this approach to the optimization of Helmholtz free energy, and following this, we also utilize it in the context of our energy function. The displacement of the particle  $i$  can be calculated as follows:

$$\Delta \mathbf{x}_i = -\eta \nabla_i \epsilon \quad (12)$$

where  $\eta$  denotes the diffusion coefficient which is used to limit the displacement of particles and mitigate artifacts such as excessive shifting and unphysical jumps. The term  $\nabla_i \epsilon$  can be computed as the derivative of the energy function  $\epsilon_i$  with respect to position  $\mathbf{x}_i$ :

$$\nabla_i \epsilon = \frac{\mathbf{x}_i - \mathbf{x}_i^*}{d_0^2} + \nabla_i E \quad (13)$$

According to Equation (6a) to Equation (10), and  $\nabla_i E$  can be expressed as follows:

$$\begin{aligned} \nabla_i E = & \nabla_i(\sigma^{LG} A^{LG}) + \nabla_i(\sigma^{LL^*} A^{LL^*}) + \nabla_i(\sigma_i^{LS} A_i^{LS}) \\ & + \nabla_i(\sigma^{SL} A^{SL}) + \nabla_i(\sigma^{SG} A^{SG}) \end{aligned} \quad (14)$$

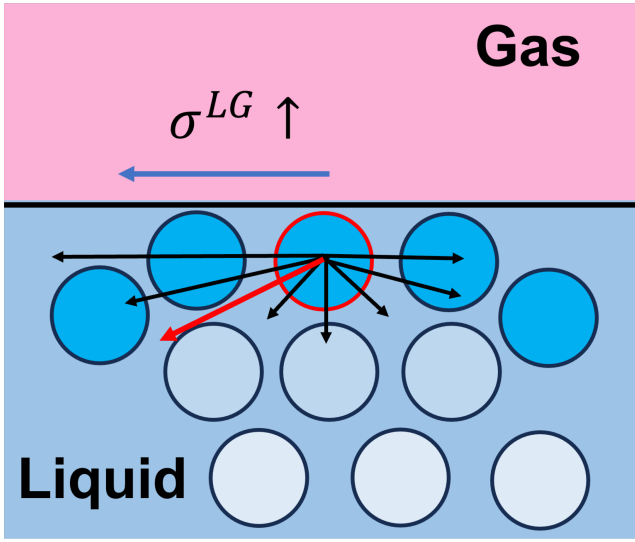
In addition to taking the derivative of the interface area, to address scenarios with non-constant tension coefficients, it is also necessary to differentiate  $\sigma$ . In conventional CSF-based tension models, the derived force is a normal force directed toward the fluid interior, which fails to capture such interfacial traction caused by variable tension coefficients. In contrast, our model inherently characterizes it, as it is fundamentally driven by energy minimization.

Since  $\tilde{C}$  is a function of  $C$ , we formally define its partial derivative with respect to  $C$  as the operator  $H$ , which can be expressed as follows:

$$H \equiv \frac{\partial}{\partial C} \tilde{C} = \frac{\max(C, 0)}{\sqrt{C^2 + \xi^2}} \quad (15)$$

Consequently, the interface energy can be discretized through a variant of SPH derivative operator [29] into the following formulation:

$$\begin{aligned} \nabla_i E = & -A_0 V_0 \sum_j (\sigma_i^{LG} H_i + \sigma_j^{LG} H_j) \nabla W_{ij} \\ & - A_0 \sum_b (V_b \sigma_i^{LG} H_i + V_0 \sigma_b^{SG} H_b) \nabla W_{ib} \\ & + A_0 V_0 \sum_{j \notin L} (\sigma_i^{LL^*} H_i + \sigma_j^{LL^*} H_j) \nabla W_{ij} \\ & + A_0 \sum_b (V_b \sigma_i^{LS} H_i + V_0 \sigma_b^{SL} H_b) \nabla W_{ib} \end{aligned} \quad (16)$$



**FIGURE 2** | Tension effect with spatial gradients. The particles are primarily influenced by neighboring particles that are close to the interface, and their behavior is more significantly affected by regions with high surface tension.

It can be observed that only particles adjacent to the interface exhibit pronounced  $H$  values. Therefore, according to Equation (16), the contribution arises only from particles at the interface. This behavior is consistent with macroscopic physical descriptions and eliminates the need to compute the interfacial spatial gradient of  $\sigma$  [12]. Figure 2 illustrates the effect of our computation.

We revisit the diffusion coefficient  $\eta$  in Equation (12), whose value must ensure that the particle displacement in a single iteration does not become excessively large. To this end, we set an upper bound  $d_0$  on the displacement per iteration, and thus  $\eta$  must satisfy the following condition:

$$\eta \|\nabla \varepsilon\| \leq d_0 \quad (17)$$

By noting that

$$\|\nabla \varepsilon\| \leq \frac{\|\mathbf{x}_i - \mathbf{x}_i^*\|}{d_0^2} + \|\nabla_0 E\| \leq \frac{1}{d_0} + 2\sigma_0 A_0 \|\nabla_0 \langle 1 \rangle\| \quad (18)$$

where  $\|\nabla_0 E\|$  is a reference value that represents the upper bound of  $\|\nabla E\|$ ,  $\sigma_0$  is the upper limit of  $\sigma$ , and  $\|\nabla_0 \langle 1 \rangle\|$  is the upper limit of  $\|\nabla \langle 1 \rangle\|$  which can be computed analytically. Therefore, we define  $\eta$  as:

$$\eta = \frac{d_0}{1/d_0 + 2\sigma_0 A_0 \|\nabla_0 \langle 1 \rangle\|} \quad (19)$$

## 5 | Implementation

Within SPH frameworks, the precision of kernel estimation is critically dependent on the number of particles within the support domain. This dependency becomes especially significant in

surface tension calculations, where the absence of sufficient particles near the interface severely degrades computational accuracy. To address this issue, we adopted an enlarged support radius for tension calculation, which is determined as  $h^{st} = 3d_0$ .

Although we treat the tension coefficient as a variable, the underlying determinants governing its parametric variation remain undefined. Factors such as liquid concentration and temperature can affect the magnitude of the tension coefficient. Considering computational complexity, our iterative solution scheme does not update the tension coefficient at every iteration step, but rather maintains it as an independent process.

For the implementation of the whole fluid system, we adopt an operator splitting strategy, where surface tension, viscous forces, external forces, and pressure are sequentially solved. To enforce fluid incompressibility, we developed a pressure solver based on IISPH [30], which was subsequently adapted for multiphase flow simulation [31]. Solids are also discretized by particles, and we use the method proposed by Band et al. [32] for fluid-solid coupling. The simulation process in a time step is shown in Algorithm 1.

### ALGORITHM 1 | Simulation loop.

---

```

1: Neighbor searching with two support radius  $h$  and  $h^{st}$ 
2: for all solid particles  $b$  do
3:   Compute volume  $V_b$  ▷ Equation (2)
4: end for
5: for all fluid particles  $i$  do
6:    $\mathbf{x}^* \leftarrow \mathbf{x}$  ▷ Store original positions
7: end for
8: while  $iter < iter_{max}$  do
9:   for all fluid particles  $i$  do
10:    Compute  $C_i$  for all interfaces ▷ Equation (7a)
to Equation (7c)
11:    Compute  $H_i \equiv \frac{\partial}{\partial C} \tilde{C}_i$  ▷ Equation (15)
12:   end for
13:   for all solid particles  $b$  do
14:    Compute  $C_b$  for all interfaces ▷ Equation (8a)
to Equation (8b)
15:    Compute  $H_b \equiv \frac{\partial}{\partial C} \tilde{C}_b$  ▷ Equation (15)
16:   end for
17:   for all particles  $i$  do
18:    Compute  $\nabla_i \varepsilon$  ▷ Equation (13) and Equation (16)
19:    Shift particles  $\mathbf{x}_i \leftarrow \eta_i \nabla_i \varepsilon$ 
20:   end for
21:    $iter = iter + 1$ 
22: end while
23: Update tension coefficient
24: Solve other forces with IISPH 30

```

---

## 6 | Results

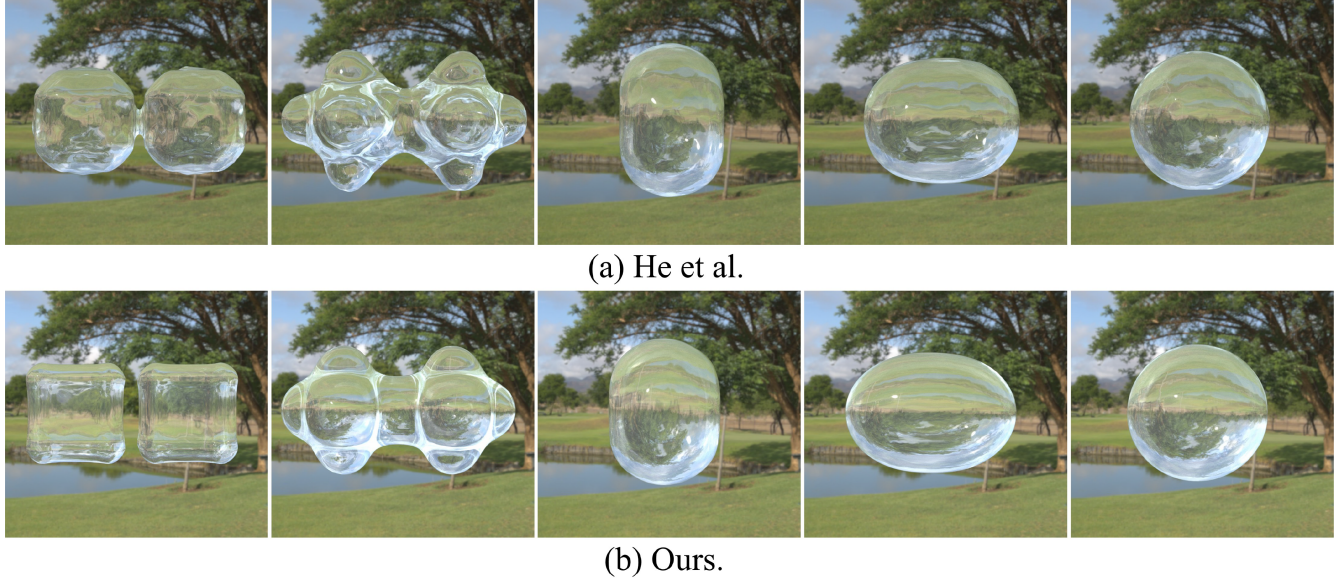
We implemented our method with C++ and parallelized the algorithm with CUDA. All simulations were performed on an Intel Core i7-12700H CPU and an Nvidia GeForce RTX 3070 Ti Laptop GPU. We used the technique proposed by Böttcher et al. [33] for surface reconstruction, Houdini and Mantra for ray tracing rendering. Table 1 shows the performance of selected examples.



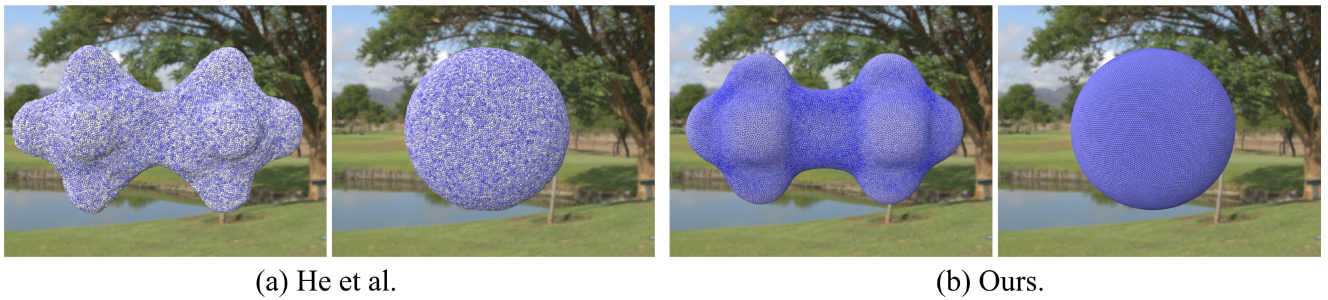
**TABLE 1** | Performance of selected examples.

| Example                                          | Particle num | Iters/step | Avg. time (s/frame) |
|--------------------------------------------------|--------------|------------|---------------------|
| Figure 3 coalescence and oscillation             | 240 k        | 15         | 18.5                |
| Figure 5 droplet impact ( $\sigma^{LG} = 5000$ ) | 65 k         | 20         | 8.7                 |
| Figure 6 contact angle ( $\theta = 180^\circ$ )  | 65 k         | 15         | 6.9                 |
| Figure 7 capillary (hydrophilic)                 | 387 k        | 10         | 14.8                |
| Figure 8 marangoni effect                        | 242 k        | 5          | 11.4                |

Note: For all examples, the frame per second (FPS) is set to 60.



**FIGURE 3** | Two liquid blocks coalesce and oscillate in zero-gravity environment. Simulation results of He et al.'s method [19] have obvious undulations on the surface, while the surface simulated by our method maintains smoothness and forms a perfect sphere. Frames 1, 10, 70, 140, and 350 are shown from left to right.



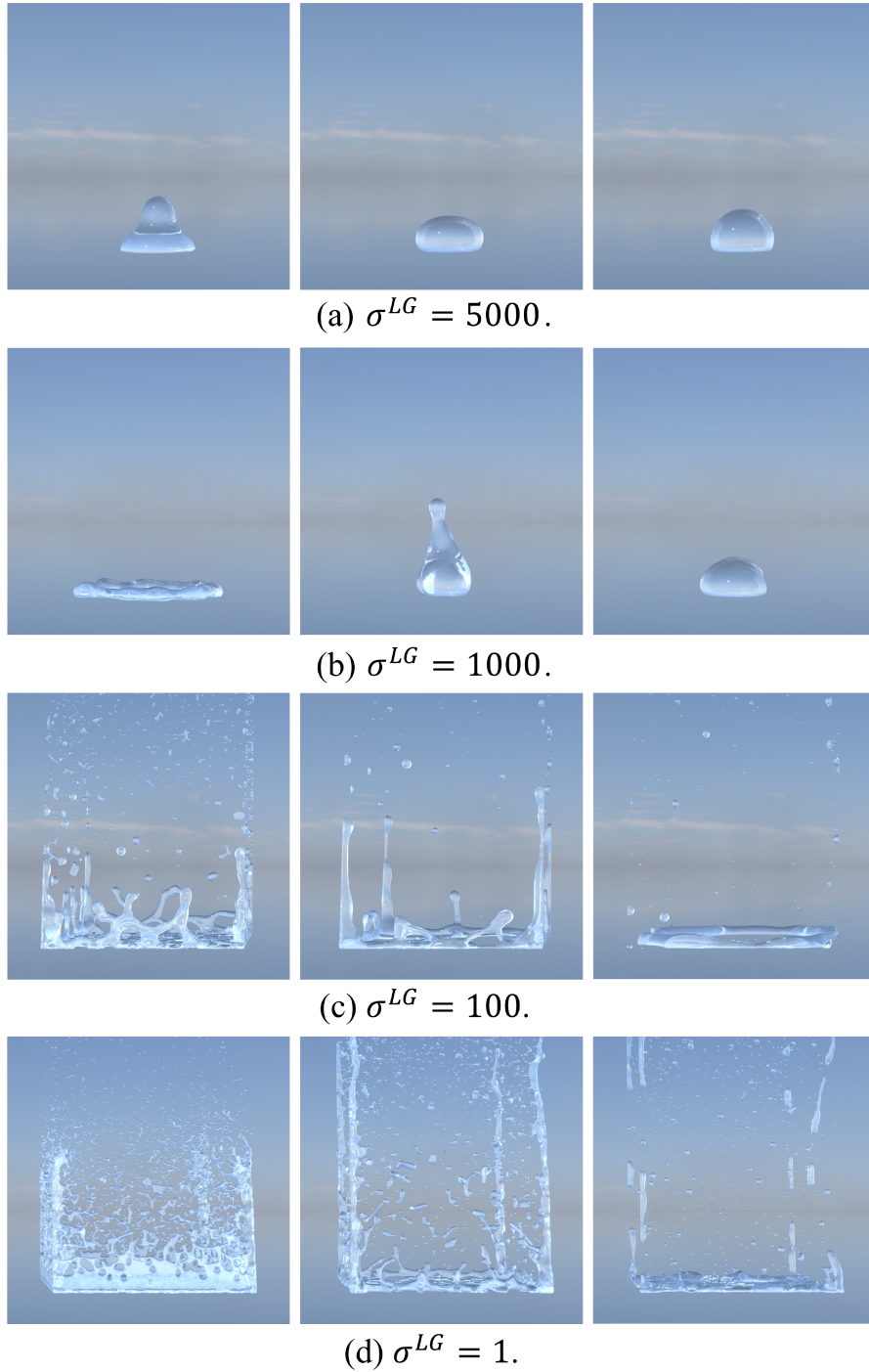
**FIGURE 4** | Schematic of particle view with velocity magnitude color-coding, where white denotes higher velocity values and blue indicates lower velocity. Frames 10 and 350 are shown.

## 6.1 | Coalescence and Oscillation

We conducted a coalescence and oscillation experiment with dual cubic water coalesces to assess the numerical accuracy and stability of our methodology. Initialized in a zero-gravity environment, the system demonstrated progressive fluidic deformation leading to complete coalescence, followed by damped oscillations converging to hydrostatic equilibrium. The side length of a cube is set to 0.3 m, and we set a large tension coefficient  $\sigma^{LG} = 1000$ .

We conducted a comparative analysis between our method and the energy-based approach proposed by He et al. [19], with both employing the same support radius. The results are shown in Figure 3. It can be observed that the method proposed by He et al. [19] successfully achieves coalescence into a spherical form, yet the resultant surface exhibits noticeable depressions and intensified undulations. In contrast, our simulation methodology maintains surface smoothness throughout the process, ultimately forming a geometrically perfect sphere. Figure 4 shows the velocity magnitudes of surface particles at the beginning and final





**FIGURE 5** | Scene of large droplets with different tension coefficients at liquid–gas interface falling from the same height and impacting the ground. The physical times from left to right are 0.16, 0.36, and 1.00 s, respectively.

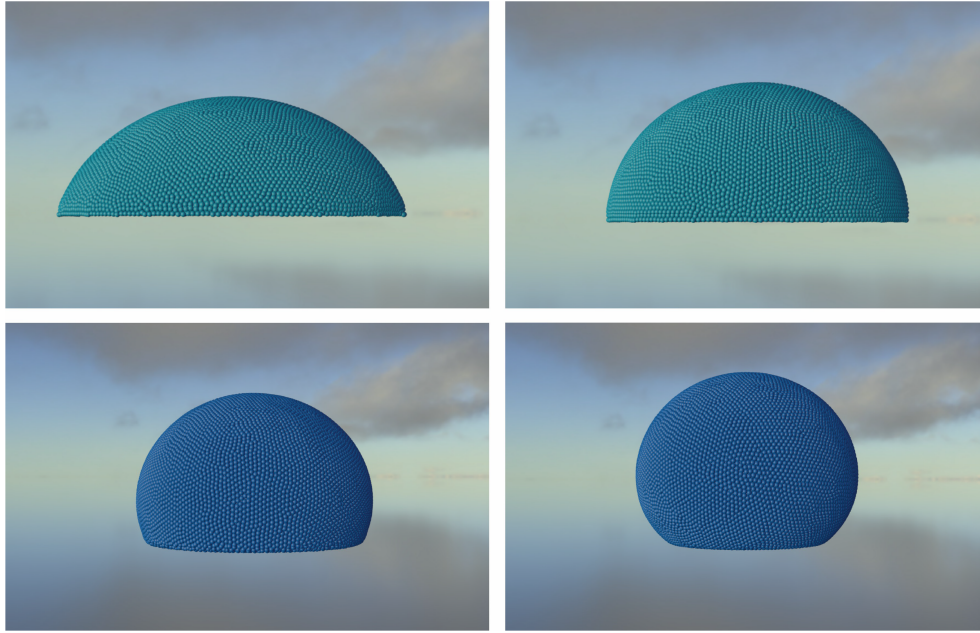
stages of the simulation. As illustrated in Figure 4a, the extremely uneven velocity of surface particles indicates significant instability in He’s method under this configuration. To compare with, Figure 4b shows a smooth velocity magnitude distribution with our method.

## 6.2 | Droplet Impact

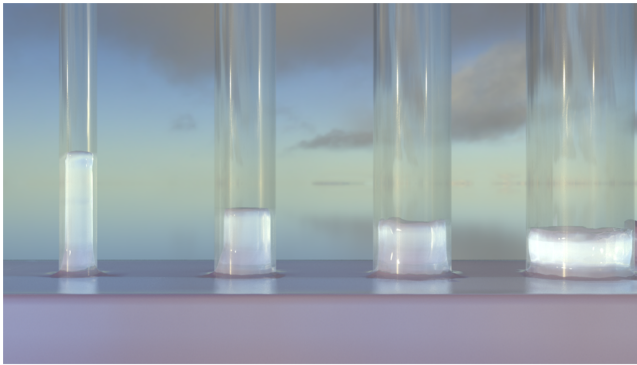
In this scenario, a spherical droplet with a diameter of 0.15 m is placed in a rectangular hydrophobic container (height: 3 m, base:

1m × 1 m), subjecting it to free fall from a height of 2.5 m. When the tension coefficients of the liquid–gas interfaces  $\sigma^{LG}$  differ, the droplet exhibited distinct behaviors after impacting the container. The results, displayed starting from the frame immediately after the droplet impacted the base, are presented in Figure 5.

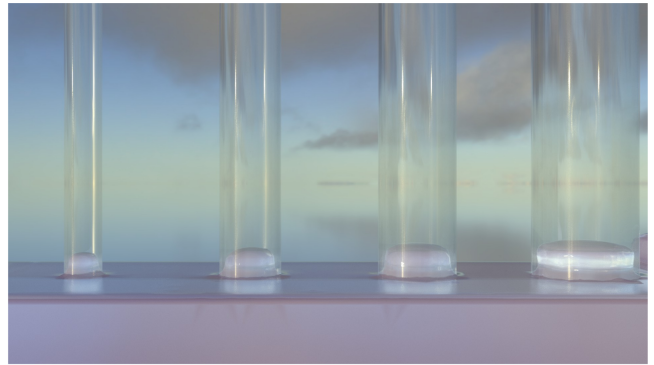
In this scenario, surface tension coefficients ranging from 1 to 5000 are simulated. It can be observed that our model demonstrates robust capability in accommodating tension coefficients spanning multiple orders of magnitude while maintaining simulation stability under such an extremely intense scenario.



**FIGURE 6** | Simulation of different contact angles. Contact angles of approximately 60°, 90°, 120°, and 180° are simulated respectively.



(a) Hydrophilic test tubes.



(b) Hydrophobic test tubes.

**FIGURE 7** | Scene of the capillary effect in test tubes. Under capillary action, hydrophilic tubes exhibit increasing water column height with decreasing tube diameter, whereas the hydrophobic tubes demonstrate suppressed liquid column formation, showing reduced water column height as tube diameter diminishes.

### 6.3 | Contact Angle

The contact angle  $\theta$  is the angle formed at the interface where a liquid meets a solid surface, measured through the liquid phase. It quantifies a liquid's wettability on a solid. Young's equation [34] describes the force balance at the three-phase (solid–liquid–gas) contact line:

$$\sigma^{SG} = \sigma^{SL} + \sigma^{LG} \cos \theta \quad (20)$$

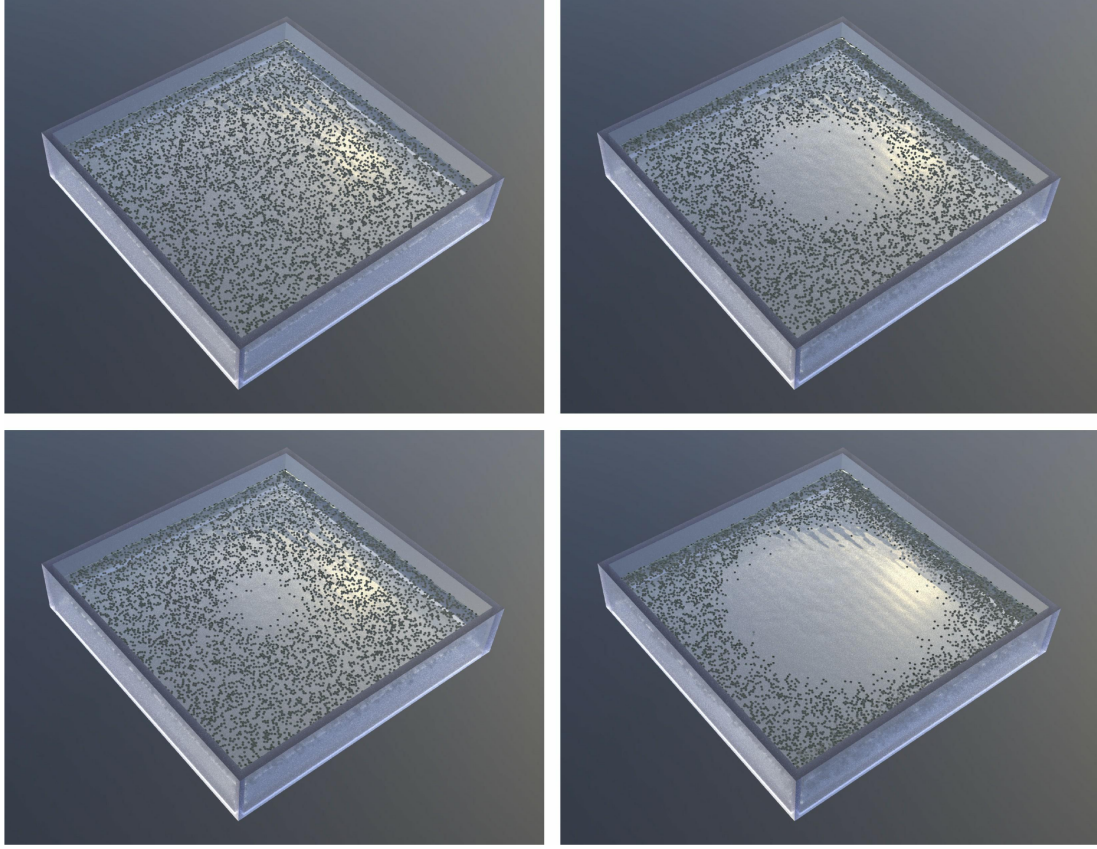
In contrast to Chen et al.'s method [23], our model enables direct customization of contact angles through Young's equation, eliminating the necessity for parametric omission. In this scenario, we set up a spherical water block with a diameter of 0.12 m near the ground, which gradually stabilized after a brief oscillation. The tension coefficient of the liquid–gas interface is set at 5000, and the tension coefficients of the ground material are determined using Young's equation with preset contact angles: 60°, 90°, 120°, and 180°.

Figure 6 presents the results of the experiment, where it is evident that the simulated contact angle closely matches the preset value.

### 6.4 | Capillary Effect

Capillary effect is the ability of a liquid to flow in narrow spaces or tubes driven by interface forces, often against gravity. When a liquid adheres strongly to a tube's material, it climbs upward, forming a concave meniscus. In contrast, if the liquid–gas interface dominates, the liquid is depressed, creating a convex meniscus. Our model naturally captures this behavior with the unified interface energy description.

As shown in Figure 7, four test tubes with varying diameters are inserted into the water surface. We set  $\sigma^{LG}$  to 1. Figure 7a



**FIGURE 8** | A classic case of the Marangoni effect. The surface tension in the center of the pool is reduced by surfactant. The spatial gradients of tension drive the small debris on the surface to move to the walls of the container. Frames 0, 10, 20, and 40 are shown in this figure.

illustrates the experimental results for hydrophilic test tubes with  $\sigma^{SL} = 0$  and  $\sigma^{SG} = 2$ . In order to reduce interface energy, the water column in test tubes rises against gravity to cover more liquid–gas interface area. Under the influence of gravity, narrower test tubes enable the liquid column to climb to higher heights. In Figure 7b the tension coefficients are set to  $\sigma^{SL} = 2$  and  $\sigma^{SG} = 0$ . The liquid column is pushed, forming a convex meniscus.

### 6.5 | Marangoni Effect

We demonstrate the tension gradients driven flow by simulating how soap reduces the surface tension of water which is a classic case of the Marangoni effect. For simplicity, we designate a subset of the SPH particles at the surface of a shallow water pool to serve as proxies for debris, and initialize a region at the center of the pool as the soap area. The surrounding water gradually becomes influenced by the soap region. Here, we implement a simple concentration diffusion model to simulate the spread of soapy water, where the surface tension coefficient decreases linearly with the soap concentration. The coefficient  $\sigma^{LG}$  of pure water is set to 10, and the minimum is set to 0.5.

Due to the spatial gradient in surface tension along the interface, particles spontaneously flow from regions of lower surface tension to regions of higher surface tension. As illustrated in Figure 8, the marked particles on the liquid surface rapidly diffuse

from the center driven by spatial gradients of tension. This indicates that our model has successfully captured this phenomenon.

## 7 | Conclusion

In this paper, we propose a tension model based on the interface energy for particle-based fluid simulation. The energy density function is minimized via an energy diffusion-driven particle displacement scheme in several iterations, which holistically balances inertia and interface energy. This method demonstrates computational efficiency while capturing versatile interfacial phenomena, including high surface tension coefficients, hydrophilic/hydrophobic effects, capillary, and more. Crucially, our formulation inherently incorporates spatial gradients of surface tension coefficients, a factor frequently overlooked in prior tension modeling techniques. Our unified derivation enables spontaneous simulations of the Marangoni effect, where particles migrate along interfaces under tension differentials without requiring explicit interfacial spatial gradient computations [12].

Nevertheless, our work still has many limitations. First, following the recommendation of Yang et al. [6], we increased the support radius during surface tension computation, which significantly increased the computational cost. A more advanced interface estimation method could potentially alleviate this dependency. Furthermore, while our energy diffusion method has achieved promising results, it remains constrained by the time



step and lacks momentum conservation. A more rigorous implicit energy optimization framework is needed to address these issues. Finally, the development of a unified solver framework presents an intriguing research frontier, particularly given its demonstrated advantages in related works [24]. We aspire to integrate other fluid phenomena and fluid-solid two-way coupling within a unified energy-based framework.

## Author Contributions

**Qianwei Wang:** writing – original draft, validation, methodology, software, visualization, conceptualization. **Yanrui Xu:** writing – review and editing, validation. **Xiangyu Sheng:** visualization, validation. **Chao Yao:** supervision, investigation. **Yu Guo:** supervision, investigation. **Jian Chang:** supervision, investigation. **Jianjun Zhang:** supervision, investigation. **Xiaokun Wang:** supervision, resources, writing – review and editing, funding acquisition

## Acknowledgments

This research is supported by Basic and Applied Basic Research Foundation of Guangdong Province (Grant No. 2023A1515030177), National Natural Science Foundation of China (Nos. 62376025, 62332017), Key Research and Development Project of Hainan Province (ZDYF2024GXJS032), National High Level Hospital Clinical Research Funding (2022-PUMCH-D-004).

## Disclosure

The authors have nothing to report.

## Conflicts of Interest

The authors declare no conflicts of interest.

## Data Availability Statement

Data sharing not applicable to this article as no datasets were generated or analyzed during the current study.

## References

1. N. Akinci, G. Akinci, and M. Teschner, “Versatile Surface Tension and Adhesion for SPH Fluids,” *ACM Transactions on Graphics* 32, no. 6 (2013): 1–8, <https://doi.org/10.1145/2508363.2508395>.
2. M. Becker and M. Teschner, “Weakly Compressible SPH for Free Surface Flows,” in *Eurographics/SIGGRAPH Symposium on Computer Animation*, ed. D. Metaxas and J. Popovic (Eurographics Association, 2007).
3. H. Wang, Y. Jin, A. Luo, X. Yang, and B. Zhu, “Codimensional Surface Tension Flow Using Moving-Least-Squares Particles,” *ACM Transactions on Graphics* 39, no. 4 (2020): 1–14, <https://doi.org/10.1145/3386569.3392487>.
4. F. Da, C. Batty, C. Wojtan, and E. Grinspun, “Double Bubbles Sans Toil and Trouble: Discrete Circulation-Preserving Vortex Sheets for Soap Films and Foams,” *ACM Transactions on Graphics* 34, no. 4 (2015): 1–9, <https://doi.org/10.1145/2767003>.
5. S. Ishida, M. Yamamoto, R. Ando, and T. Hachisuka, “A Hyperbolic Geometric Flow for Evolving Films and Foams,” *ACM Transactions on Graphics* 36, no. 6 (2017): 1–11, <https://doi.org/10.1145/3130800.3130835>.
6. T. Yang, R. R. Martin, M. C. Lin, J. Chang, and S. M. Hu, “Pairwise Force SPH Model for Real-Time Multi-Interaction Applications,” *IEEE Transactions on Visualization and Computer Graphics* 23, no. 10 (2017): 2235–2247, <https://doi.org/10.1109/TVCG.2017.2706289>.

7. T. Probst and M. Teschner, “Unified Pressure, Surface Tension and Friction for SPH Fluids,” *ACM Transactions on Graphics* 44, no. 1 (2024): 1–28, <https://doi.org/10.1145/3708034>.
8. L. Ruan, J. Liu, B. Zhu, S. Sueda, B. Wang, and B. Chen, “Solid-Fluid Interaction With Surface-Tension-Dominant Contact,” *ACM Transactions on Graphics* 40, no. 4 (2021): 1–12, <https://doi.org/10.1145/3450626.3459862>.
9. X. K. Wang, X. J. Ban, Y. L. Zhang, S. N. Liu, and P. F. Ye, “Surface Tension Model Based on Implicit Incompressible Smoothed Particle Hydrodynamics for Fluid Simulation,” *Journal of Computer Science and Technology* 32 (2017): 1186–1197.
10. L. Yang, M. Rakhsha, and D. Negrut, “Comparison of Surface Tension Models in Smoothed Particles Hydrodynamics Method,” in *International Design Engineering Technical Conferences and Computers and Information in Engineering Conference*. American Society of Mechanical Engineers, vol. 59261 (The American Society of Mechanical Engineers, 2019), V006T09A028.
11. S. R. Jeske, L. Westhofen, F. Löschner, J. A. Fernández-fernández, and J. Bender, “Implicit Surface Tension for SPH Fluid Simulation,” *ACM Transactions on Graphics* 43, no. 1 (2023): 1–14, <https://doi.org/10.1145/3631936>.
12. M. Tong and D. J. Browne, “An Incompressible Multi-Phase Smoothed Particle Hydrodynamics (SPH) Method for Modelling Thermocapillary Flow,” *International Journal of Heat and Mass Transfer* 73 (2014): 284–292.
13. S. Bouaziz, S. Martin, T. Liu, L. Kavan, and M. Pauly, “Projective Dynamics: Fusing Constraint Projections for Fast Simulation,” *ACM Transactions on Graphics* 33, no. 4 (2014): 1–11, <https://doi.org/10.1145/2601097.2601116>.
14. N. Akinci, M. Ihmsen, G. Akinci, B. Solenthaler, and M. Teschner, “Versatile Rigid-Fluid Coupling for Incompressible SPH,” *ACM Transactions on Graphics* 31, no. 4 (2012): 1–8, <https://doi.org/10.1145/2185520.2185558>.
15. M. Huber, S. Reinhardt, D. Weiskopf, and B. Eberhardt, “Evaluation of Surface Tension Models for SPH-Based Fluid Animations Using a Benchmark Test,” in *Workshop on Virtual Reality Interaction and Physical Simulation*, ed. F. Jallet, F. Zara, and G. Zachmann (Eurographics Association, 2015), 41–50.
16. J. Brackbill, D. Kothe, and C. Zemach, “A Continuum Method for Modeling Surface Tension,” *Journal of Computational Physics* 100, no. 2 (1992): 335–354, [https://doi.org/10.1016/0021-9991\(92\)90240-Y](https://doi.org/10.1016/0021-9991(92)90240-Y).
17. J. P. Morris, “Simulating Surface Tension With Smoothed Particle Hydrodynamics,” *International Journal for Numerical Methods in Fluids* 33, no. 3 (2000): 333–353.
18. S. Adami, X. Hu, and N. Adams, “A New Surface-Tension Formulation for Multi-Phase SPH Using a Reproducing Divergence Approximation,” *Journal of Computational Physics* 229, no. 13 (2010): 5011–5021, <https://doi.org/10.1016/j.jcp.2010.03.022>.
19. X. He, H. Wang, F. Zhang, H. Wang, G. Wang, and K. Zhou, “Robust Simulation of Sparsely Sampled Thin Features in SPH-Based Free Surface Flows,” *ACM Transactions on Graphics* 34, no. 1 (2015): 1–9, <https://doi.org/10.1145/2682630>.
20. F. Da, D. Hahn, C. Batty, C. Wojtan, and E. Grinspun, “Surface-Only Liquids,” *ACM Transactions on Graphics* 35, no. 4 (2016): 1–12, <https://doi.org/10.1145/2897824.2925899>.
21. J. Xing, L. Ruan, B. Wang, B. Zhu, and B. Chen, “Position-Based Surface Tension Flow,” *ACM Transactions on Graphics* 41, no. 6 (2022): 1–12, <https://doi.org/10.1145/3550454.3555476>.
22. D. A. B. Hyde, S. W. Gagniere, A. Marquez-Razon, and J. Teran, “An Implicit Updated Lagrangian Formulation for Liquids With Large Surface Energy,” *ACM Transactions on Graphics* 39, no. 6 (2020): 1–13, <https://doi.org/10.1145/3414685.3417845>.



23. J. Chen, V. Kala, A. Marquez-Razon, E. Gueidon, D. A. B. Hyde, and J. Teran, “A Momentum-Conserving Implicit Material Point Method for Surface Tension With Contact Angles and Spatial Gradients,” *ACM Transactions on Graphics* 40, no. 4 (2021): 1–16, <https://doi.org/10.1145/3450626.3459874>.
24. T. Takahashi and C. Batty, “Frictional Monolith: A Monolithic Optimization-Based Approach for Granular Flow With Contact-Aware Rigid-Body Coupling,” *ACM Transactions on Graphics* 40, no. 6 (2021): 1–20.
25. J. Monaghan, “Simulating Free Surface Flows With SPH,” *Journal of Computational Physics* 110, no. 2 (1994): 399–406.
26. M. Brugger, R. Traxl, and R. Lackner, “Energy-Conserving Formulation of the CSF Model for the Simulation of Surface Tension at Fluid-Fluid Interfaces With Smoothed Particle Hydrodynamics,” *Journal of Computational Physics* 476 (2023): 111895, <https://doi.org/10.1016/j.jcp.2022.111895>.
27. S. Lind, R. Xu, P. Stansby, and B. Rogers, “Incompressible Smoothed Particle Hydrodynamics for Free-Surface Flows: A Generalised Diffusion-Based Algorithm for Stability and Validations for Impulsive Flows and Propagating Waves,” *Journal of Computational Physics* 231, no. 4 (2012): 1499–1523, <https://doi.org/10.1016/j.jcp.2011.10.027>.
28. X. He, H. Wang, G. Wang, H. Wang, and E. Wu, “A Variational Staggered Particle Framework for Incompressible Free-Surface Flows,” 2020.
29. A. Colagrossi and M. Landrini, “Numerical Simulation of Interfacial Flows by Smoothed Particle Hydrodynamics,” *Journal of Computational Physics* 191, no. 2 (2003): 448–475.
30. M. Ihmsen, J. Cornelis, B. Solenthaler, C. Horvath, and M. Teschner, “Implicit Incompressible SPH,” *IEEE Transactions on Visualization and Computer Graphics* 20, no. 3 (2014): 426–435, <https://doi.org/10.1109/TVCG.2013.105>.
31. B. Solenthaler and R. Pajarola, “Density Contrast SPH Interfaces,” in *Eurographics/SIGGRAPH Symposium on Computer Animation*, ed. M. Gross and D. James (Eurographics Association, 2008).
32. S. Band, C. Gissler, M. Ihmsen, J. Cornelis, A. Peer, and M. Teschner, “Pressure Boundaries for Implicit Incompressible SPH,” *ACM Transactions on Graphics* 37, no. 2 (2018): 1–11.
33. F. Löffner, T. Böttcher, S. R. Jeske, and J. Bender, “Weighted Laplacian Smoothing for Surface Reconstruction of Particle-Based Fluids,” in *Vision, Modeling, and Visualization* (Eurographics Association, 2023).
34. T. Young, “An Essay on the Cohesion of Fluids,” *Philosophical Transactions of the Royal Society of London Series I* 95 (1805): 65–87.

## Supporting Information

Additional supporting information can be found online in the Supporting Information section. **Video S1.** Supporting Information.