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Numerical Method for The Simulation of Contact Angle Dynamics

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Abstract. In this research, we develop a method to simulate nonsymmetric triple junction motion given by the gradient flow of surface energy with arbitrary surface tensions of the participating interfaces. The foundation of the method is the diffusion-based BMO algorithm in vector-valued formulation. We realize the nonsymmetric motion by generalizing the original BMO method and adding a corrective projection step. In the end, we show the numerical example for the simulation of the bubble motion using two different contact angles to simulate the contact angle dynamics.

INTRODUCTION

Understanding the contact angle dynamics is very useful to realize some kinds of important phenomena. An example of such phenomena is the motion of small droplets or bubbles which has important applications in nanotechnology and heat transfer.

In this research, we develop an interface model with contact angle. The interface between two fluids is considered as a membrane with its own physical parameters. We build an interface model based on gradient flow of surface energy and develop a numerical model for interface motion with arbitrary surface tensions leading to nonsymmetric triple junctions. To treat such curvature-dependent motions, several methods have been developed. For symmetric junctions, Merriman, Bence and Osher [1] introduced the BMO method, which alternately diffuses and sharpens characteristic function for each phase region. Ruuth [2] generalized the BMO method to nonsymmetric triple junctions by replacing the thresholding step with a new decision using a projection triangle. Svadlenka et al. [3] reformulated the BMO algorithm in a vector-valued setting for multiphase motion. This vector-valued formulation is essential for implementing constraints and for dealing with more general motions. However, it is restricted to the symmetric case. Mohammad et al. [4] improved the symmetric multiphase BMO algorithm of [3] by introducing a vector-valued signed distance function.

In this work, we consider three evolving curves meeting at a junction and having arbitrary surface tensions. We achieve the simulation of such a triple junction by generalizing the two main ingredients of the method in [3]: the reference vectors (corresponding to the positions of wells in the phase-field method) and the way of diffusing. Moreover, we improve the scheme by including a modification of the projection step in [2]. The developed method is applicable to constrained motions, which is essential for the considered coupled model. The contact angle dynamics have been analyzed using interface-fluid coupled model that have been developed in [5, 6].

BASIC MODEL

Interface Model: Equations of Triple Junction

We consider three evolving curves $\gamma_i(s)$, $s \in [p_i, q_i]$, $i = 1, 2, 3$, which lie inside a fixed smooth region Ω of $\mathbb{R}^2$, meet the outer boundary $\partial\Omega$ at a right angle and get together at a triple junction $x_T = \gamma_i(q_i)$, $i = 1, 2, 3$. Each curve has different surface tension σ_i .

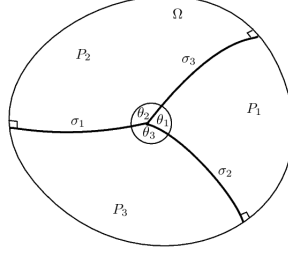


FIGURE 1. Triple junction

Then the surface energy of all curves is given by

$$L(\gamma) = \sum_{i=1}^3 \int_{\gamma_i} \sigma_i \, dl = \sum_{i=1}^3 \int_{p_i}^{q_i} \sigma_i |\gamma'_i(s)| \, ds.$$

Define the tangential vector t_i , curvature κ_i and outer normal n_i of curve γ_i by

$$t_i = \frac{\gamma'_i}{|\gamma'_i|}, \quad \kappa_i = -\frac{\gamma'_{ix}\gamma''_{iy} - \gamma'_{iy}\gamma''_{ix}}{|\gamma'_i|^3}, \quad n_i = \frac{1}{|\gamma'_i|}(\gamma'_{iy}, -\gamma'_{ix}).$$

For a smooth vector field φ vanishing near the boundary $\partial\Omega$, the gradient flow of surface energy can be found from its variation,

$$\begin{aligned} \frac{d}{d\epsilon} L(\gamma + \epsilon\varphi(\gamma))|_{\epsilon=0} &= \sum_{i=1}^3 \int_{p_i}^{q_i} \sigma_i t_i \cdot \frac{d}{ds}(\varphi(\gamma_i)) \, ds \\ &= \sum_{i=1}^3 \left(- \int_{\gamma_i} (\sigma_i \kappa_i n_i) \cdot \varphi \, dl + \sigma_i t_i \cdot \varphi(x_T) \right). \end{aligned}$$

From this result, the motion by gradient flow satisfies

$$\text{The normal velocity of interface: } v_i = \sigma_i \kappa_i. \tag{1}$$

$$\text{Condition at triple junction: } \sum_{i=1}^3 \sigma_i t_i = 0. \tag{2}$$

The junction condition (2) is the balance of forces which is well-known to be equivalent to the Young's law

$$\frac{\sin \theta_1}{\sigma_1} = \frac{\sin \theta_2}{\sigma_2} = \frac{\sin \theta_3}{\sigma_3},$$

where $\theta_1, \theta_2, \theta_3$ are the stable angles. This yields

$$\begin{cases} \cos(\pi - \theta_1) = \frac{\sigma_3^2 + \sigma_2^2 - \sigma_1^2}{2\sigma_2\sigma_3}, \\ \cos(\pi - \theta_2) = \frac{\sigma_1^2 + \sigma_3^2 - \sigma_2^2}{2\sigma_1\sigma_3}, \\ \theta_1 + \theta_2 + \theta_3 = 2\pi. \end{cases} \tag{3}$$

Note that we can compute the stable angles with any given triple of surface tensions, as long as the triple satisfies the triangle inequality.

NUMERICAL METHOD

Interface Model: BMO Algorithm with Arbitrary Surface Tensions

Vector-valued BMO

The basis of our method is the vector-valued BMO algorithm [3]:

1. Define symmetric reference vectors $\mathbf{p}_i$ of dimension two, each corresponding to a phase P_i for $i = 1, 2, 3$.
2. Given a partition P_i , $i = 1, 2, 3$, set $\mathbf{u}_0(x) = \mathbf{p}_i$ for $x \in P_i$.
3. Repeat
 - Solve the vector-valued heat equation with initial condition $\mathbf{u}_0$:

$$\mathbf{u}_t(t, x) = \Delta \mathbf{u}(t, x) \quad \text{for } (t, x) \in (0, \Delta t] \times \Omega,$$

$$\frac{\partial \mathbf{u}}{\partial \mathbf{n}}(t, x) = 0 \quad \text{on } (0, \Delta t] \times \partial \Omega.$$

- Update $\mathbf{u}_0$ by identifying the reference vector which is closest to the solution $\mathbf{u}(\Delta t, x)$:

$$\mathbf{u}_0(x) = \mathbf{p}_j,$$

$$\text{where } \mathbf{p}_j \cdot \mathbf{u}(\Delta t, x) = \max_{i=1,2,3} \mathbf{p}_i \cdot \mathbf{u}(\Delta t, x).$$

This redistribution of reference vectors determines the configuration of phases after time Δt .

The paper [3] deals only with symmetric junctions and therefore, the above algorithm works with symmetric reference vectors and simple heat equation in the diffusion step, as is formally proved there. However, for arbitrary junction angles, this setting is not sufficient and has to be generalized. The main ideas of this generalization were already outlined in [7, 8] and will be explained in the following subsections.

Junction Stability

We consider a stable configuration which yields a condition on the selection of reference vectors for the BMO algorithm. Here we consider three straight lines meeting at the origin with the given stable angles as in Figure 2.

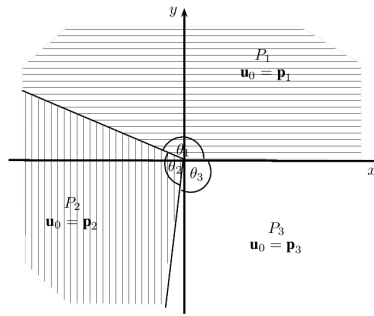


FIGURE 2. A stable junction

The triple junction does not move if $\mathbf{u}(t, 0, 0) = \mathbf{0}$ for all $t > 0$, where $\mathbf{u}$ is the solution of the heat equation,

$$\frac{1}{4\pi t} \sum_{i=1}^3 \mathbf{p}_i \int_{\mathbf{R}^2 \cap P_i} \exp\left(-\frac{x^2}{4t}\right) dx = \mathbf{0}.$$

Since the integrals can be evaluated exactly, we get

$$\theta_1 \mathbf{p}_1 + \theta_2 \mathbf{p}_2 + \theta_3 \mathbf{p}_3 = \mathbf{0}. \quad (4)$$

The above relation is a one-dimension higher BMO analogue of Young's law in the sense that the reference vectors $\mathbf{p}_i$ are distributed in the whole phase regions P_i and, thus, the equilibrium condition is related to area integrals, which results in weights equal to junction angles.

The vector equation (4) and the condition obtained in the next section that the lengths of $\mathbf{p}_i, i = 1, 2, 3$, must be equal, form a systems of equations for the components of $\mathbf{p}_i$:

$$\begin{aligned} \theta_1 p_1^1 + \theta_2 p_2^1 + \theta_3 p_3^1 &= 0 \\ \theta_1 p_1^2 + \theta_2 p_2^2 + \theta_3 p_3^2 &= 0 \\ (p_1^1)^2 + (p_1^2)^2 &= 1 \\ (p_2^1)^2 + (p_2^2)^2 &= 1 \\ (p_3^1)^2 + (p_3^2)^2 &= 1 \end{aligned}$$

Since the reference vectors are determined up to rotation and scaling, we can choose one reference vector arbitrarily, e.g., we set $\mathbf{p}_3 = (1, 0)$. This closes the system and its solution can be written as

$$\begin{cases} \mathbf{p}_1 = \left(1 - \frac{2\pi}{\theta_1 \theta_3} (\pi - \theta_2), \pm \frac{2}{\theta_1 \theta_3} \sqrt{\pi(\pi - \theta_1)(\pi - \theta_2)(\pi - \theta_3)} \right) \\ \mathbf{p}_2 = \left(1 - \frac{2\pi}{\theta_2 \theta_3} (\pi - \theta_1), \mp \frac{2}{\theta_2 \theta_3} \sqrt{\pi(\pi - \theta_1)(\pi - \theta_2)(\pi - \theta_3)} \right) \\ \mathbf{p}_3 = (1, 0) \text{ (arbitrarily fixed).} \end{cases} \quad (5)$$

Interface Velocity

We study the modification of the original BMO algorithm yielding the correct interface velocities $v_i = \sigma_i \kappa_i$. The idea is to consider the general diffusion system

$$\mathbf{u}_t = A \Delta \mathbf{u}, \quad (6)$$

with $\mathbf{u}(t = 0) = \mathbf{u}_0$, where $A = \begin{pmatrix} a & b \\ b & c \end{pmatrix}$ and determine its coefficients a, b, c , so that we obtain the desired interface velocities. We assume that A is positive definite then diagonalize it as follows,

$$A = K \Lambda K^{-1} \quad \text{with} \quad \Lambda = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}.$$

The eigenvalues of A are given by

$$\lambda_{1,2} = \frac{a + c \pm r}{2},$$

where $r = \sqrt{(a - c)^2 + 4b^2}$ and K is the matrix of eigenvectors.

The original problem is transformed into

$$\begin{cases} w_t^1 = \lambda_1 \Delta w^1, \\ w_t^2 = \lambda_2 \Delta w^2, \\ \left(w^1, w^2 \right)^T (t = 0) = \left(w_0^1, w_0^2 \right)^T \end{cases} \quad (7)$$

where $\left(w^1, w^2 \right)^T = K^{-1} \left(u^1, u^2 \right)^T$

The solution of (7) in the whole $\mathbb{R}^2$ is

$$w^i(t, x) = \frac{1}{4\pi\lambda_i t} \int_{\mathbb{R}^2} w_0^i(\xi) e^{-\frac{|x-\xi|^2}{4\lambda_i t}} d\xi, \quad i = 1, 2, \quad (8)$$

where $w_0^i|_{P_j} = ((K^{-1}\mathbf{u}_0)|_{P_j})^i = (K^{-1}\mathbf{p}_j)^i, i = 1, 2, j = 1, 2, 3$.

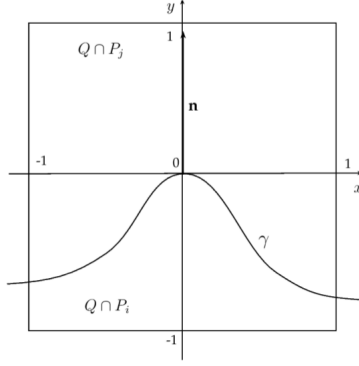


FIGURE 3. Configuration of the interface

Now, let us calculate the velocity of the interface for the above diffusion system. We consider a point on the interface $\gamma = \partial P_{ij}$ between phase P_i and P_j . We translate and rotate the coordinate system so that the chosen point lies in the origin and the outer normal at the point agrees with the positive y -direction (see Figure 3). We define $Q = [-1, 1] \times [-1, 1]$. Expressing the condition on the interface position along the y -axis after time t , the normal velocity v of the interface is

$$\mathbf{u}(t, 0, vt) \cdot (\mathbf{p}_i - \mathbf{p}_j) = 0. \quad (9)$$

The solution of the transformed problem (7) is given by

$$\mathbf{w}(t, 0, vt) = \begin{pmatrix} \frac{1}{4\pi\lambda_1 t} \int_{\mathbb{R}^2} w_0^1(\xi) e^{-\frac{|\xi - (0, vt)|^2}{4\lambda_1 t}} d\xi \\ \frac{1}{4\pi\lambda_2 t} \int_{\mathbb{R}^2} w_0^2(\xi) e^{-\frac{|\xi - (0, vt)|^2}{4\lambda_2 t}} d\xi \end{pmatrix},$$

and by the techniques in [9], we get

$$\frac{1}{4\pi\lambda_1 t} \int_{Q \cap P_i} e^{-\frac{|\xi - (0, vt)|^2}{4\lambda_1 t}} d\xi = \frac{1}{2} + \frac{\sqrt{t}}{2\sqrt{\pi\lambda_1}} (\lambda_1 \kappa - v) + O(t^{\frac{3}{2}}), \quad (10)$$

where κ is the curvature of ∂P_{ij} at the origin. Hence, we have for $l = 1, 2$, up to $O(t^{\frac{3}{2}})$,

$$w^l(t, 0, vt) = \frac{w_l^0|_{P_i} + w_l^0|_{P_j}}{2} + \frac{w_l^0|_{P_i} - w_l^0|_{P_j}}{2} \frac{\sqrt{t}}{\sqrt{\pi\lambda_l}} (\lambda_l \kappa - v).$$

We obtain from (9) the identity

$$M^{-1} \left[M \frac{\mathbf{p}_i + \mathbf{p}_j}{2} + \frac{\sqrt{t}}{\sqrt{\pi}} D M \frac{\mathbf{p}_i - \mathbf{p}_j}{2} \right] \cdot (\mathbf{p}_i - \mathbf{p}_j) = O(t^{\frac{3}{2}}),$$

where D is a diagonal matrix with $\frac{1}{\sqrt{\lambda_1}} (\lambda_1 \kappa - v)$ and $\frac{1}{\sqrt{\lambda_2}} (\lambda_2 \kappa - v)$ as diagonal elements. Notice that if the first dot product on the left-hand side does not vanish, then the order in time of the equation does not match. This leads to the condition $(\mathbf{p}_i + \mathbf{p}_j) \cdot (\mathbf{p}_i - \mathbf{p}_j) = 0$, meaning that the lengths of reference vectors have to be equal. Finally, we get the velocity of interface γ_m ,

$$v_m = -\frac{\mu_1(a + c + r) + 2\mu_2 \sqrt{ac - b^2}}{\mu_2(a + c + r) + 2\mu_1 \sqrt{ac - b^2}} \sqrt{ac - b^2} \kappa_m, \quad (11)$$

where

$$\begin{aligned} r &= \sqrt{(a - c)^2 + 4b^2} \\ \mu_1 &= [(a - c + r)(p_i^1 - p_j^1) + 2b(p_i^2 - p_j^2)]^2, \\ \mu_2 &= [2b(p_i^1 - p_j^1) - (a - c + r)(p_i^2 - p_j^2)]^2. \end{aligned}$$

From (11) and (1), we have a nonlinear system consisting of three equations for the coefficients a, b and c , which is solved numerically.

TABLE 1. Coefficients of Diffusion System in some Cases

$(\sigma_1, \sigma_2, \sigma_3)$	(a, b, c)
(1,1,1)	(1,0,1)
(1,1.5,1)	(1.43773,0.19887,0.86481)
(1.,1.8,1.)	(1.76785,0.18910,0.68793)
(1.5,0.75,1.)	(1.43308 -0.25468 0.67283)
(1.5,1.,1.)	(1.43773,-0.19887,0.86481)
(1.5,1.25,1.)	(1.50944,-0.10082,0.96859)
(1.5,2.,1.)	(2.02618,0.12516,0.89890)
(1.8,1.,1.)	(1.76785,-0.18909,0.68793)
(2.,1.5,1.)	(2.02618,-0.12516,0.89890)
(2.,2.,1.)	(2.2408,0,1)

Remark. For the initial condition in Figure 2, at the triple junction we have

$$\begin{aligned} w^i(t, 0) &= \frac{1}{4\pi\lambda_i t} \left(\int_{P_1} + \int_{P_2} + \int_{P_3} \right) w_0^i(\xi) e^{-\frac{|\xi|^2}{4\lambda_i t}} d\xi \\ &= \frac{1}{\pi} \left(\frac{\theta_1}{2} w_0^i|_{P_1} + \frac{\theta_2}{2} w_0^i|_{P_2} + \frac{\theta_3}{2} w_0^i|_{P_3} \right). \end{aligned}$$

Therefore,

$$\mathbf{w}(t, 0) = \frac{1}{2\pi} M (\theta_1 \mathbf{p}_1 + \theta_2 \mathbf{p}_2 + \theta_3 \mathbf{p}_3).$$

For junction stability, we require $\mathbf{u}(t, 0) = M^{-1} \mathbf{w}(t, 0) = \mathbf{0}$. This condition is equivalent to

$$\theta_1 \mathbf{p}_1 + \theta_2 \mathbf{p}_2 + \theta_3 \mathbf{p}_3 = \mathbf{0},$$

which is in agreement with (4).

This result shows that no matter how we change the diffusion equation, the stability condition (4) will not be affected. Hence, the selection of reference vectors can be done independently of the diffusion equation.

Correction by Projection Triangle

The above analysis does not address the close vicinity of the triple junction. Therefore, we include a correction step based on the notion of a projection triangle. The idea is to first investigate how the stable configuration of three straight lines deforms, and use this information to project the phase regions back into the correct position in each step of the BMO algorithm. See [2] for the details.

In order to relate our vector-valued formulation to the construction in [2], for $(i, j, k) \in \{(1, 2, 3), (2, 3, 1), (3, 2, 1)\}$ we introduce the functions

$$f_i(t, x) = \frac{\mathbf{u}(t, x) \cdot (\mathbf{p}_j + \mathbf{p}_k) - 1 - \mathbf{p}_j \cdot \mathbf{p}_k}{(\mathbf{p}_i - \mathbf{p}_j) \cdot (\mathbf{p}_j + \mathbf{p}_k)}. \quad (12)$$

Note that (12) is a generalization of the function $w_i(t, x)$ in [3], Section 2.2.2, for general reference vectors (5). Since $\mathbf{u}(0, x) = \mathbf{p}_i$ for $x \in P_i$, one can easily check that

$$f_i(0, x) = \chi_i(x), \quad i = 1, 2, 3,$$

where χ_i is the characteristic function of phase region P_i .

The construction of the projection triangle in the vector-valued setting is as follows:

Given an angle configuration $\theta_1, \theta_2, \theta_3$,

1. Define the lines (in polar coordinates)
 $\ell_{12} = \{(r, \frac{1}{2}\theta_1) : r > 0\}$; $\ell_{13} = \{(r, -\frac{1}{2}\theta_1) : r > 0\}$; $\ell_{23} = \{(r, \frac{1}{2}\theta_1 + \theta_2) : r > 0\}$, and regions P_1, P_2, P_3 .
2. Set $\mathbf{u}_0(x) \equiv \mathbf{p}_i$ for $x \in P_i$.
3. Apply the diffusion (6) to the initial condition $\mathbf{u}_0$ for a time $\tau \leq \Delta t$, where Δt is the BMO time step.
4. Map the values of the solution of step 3 along each line ℓ_{ij} onto the projection triangle to form the dividing lines $\tilde{\ell}_{ij} = \{\mathbf{u}(\tau, x) : x \in \ell_{ij}\}$ (Figure 4).

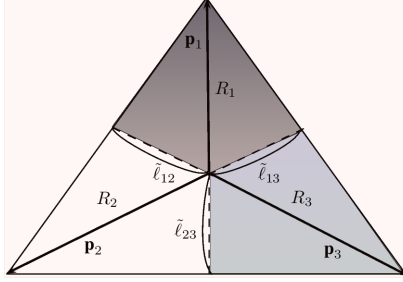


FIGURE 4. Projection triangle

The Algorithm

The generalized vector-valued BMO for three-phase motion is as follows: for given surface tensions,

1. Calculate junction angles θ_i by (3).
2. Define reference vectors $\mathbf{p}_i$ according to formula (5).
3. Find the solution a, b, c of (11) by Newton's method.
4. Construct projection triangle according to the algorithm in Section 3.1.d.
5. For a given three phase initial configuration P_1, P_2, P_3 , set $\mathbf{u}_0(x) = \mathbf{p}_i$, $x \in P_i$.
6. Repeat until desired time
 - Solve the diffusion system

$$\mathbf{u}_t = A\Delta\mathbf{u} \quad \text{for } (t, x) \in (0, \Delta t] \times \Omega, \quad (13)$$

$$\frac{\partial \mathbf{u}}{\partial \mathbf{n}} = 0 \quad \text{on } (0, \Delta t] \times \Omega,$$

$$\mathbf{u}(0, x) = \mathbf{u}_0(x) \quad \text{in } \Omega.$$

- Threshold according to the projection triangle defined in step 4, i.e.,

$$\mathbf{u}_0(x) = \mathbf{p}_i \quad \text{if } \mathbf{u}(x) \in R_i, \quad i = 1, 2, 3,$$

where R_i are the regions in Figure 4.

The modified diffusion system is solved by using vector-type discrete Morse flow (DMF), i.e., at each step we solve (13) by discretizing time $\Delta t = h \times N$ and successively minimizing the following functionals for $n = 1, \dots, N$ over $H^1(\Omega; \mathbb{R}^2)$:

$$J_n(\mathbf{u}) = \int_{\Omega} \left(\frac{a}{2} |\nabla u^1|^2 + b \nabla u^1 \cdot \nabla u^2 + \frac{c}{2} |\nabla u^2|^2 \right) dx + \int_{\Omega} \left(\frac{|\mathbf{u} - \mathbf{u}_{n-1}|^2}{2h} \right) dx. \quad (14)$$

We approximate the functional (14) by using piecewise linear finite elements. The minimizers are found by steepest descent method.

In the volume constrained case, we include the constraint via penalization, i.e., we minimize the functional

$$F_n(\mathbf{u}) = J_n(\mathbf{u}) + \frac{1}{\epsilon} \sum_{i=1}^3 |V_i - \text{meas}(P_i^{\mathbf{u}})|^2,$$

where $\epsilon > 0$ is a small penalty parameter, V_i is the prescribed volume of region P_i and the volumes corresponding to $\mathbf{u}$ are obtained from the sets $P_i^{\mathbf{u}} = \{x \in \Omega; \mathbf{u}(x) \in R_i\}$.

NUMERICAL EXAMPLE

We simulate the bubble motion with buoyancy (β) as outer force in two settings, $\theta = 60^\circ$ and $\theta = 120.1^\circ$. The numerical examples are conducted on a $[0, 1] \times [0, 1]$ domain which is triangulated into 12,800 elements, $\epsilon = 10^{-5}$, $\beta = -150$, $\delta_1 = \delta_2 = \Delta x$ (mesh size). Under the same buoyant force, we see that for a large contact angle ($\theta = 120.1^\circ$), the bubble detaches from the bottom phase, while for $\theta = 60^\circ$ the bubble remains attached (Figure 5).

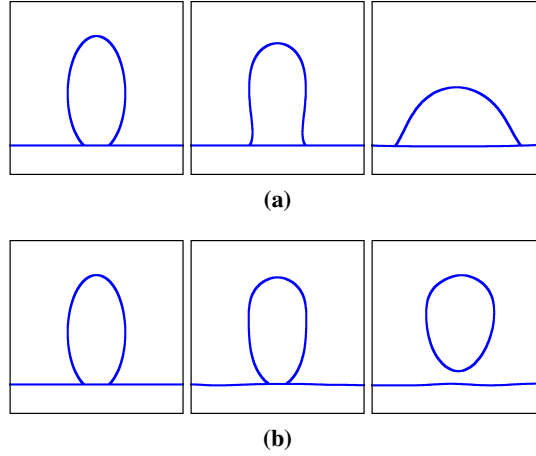


FIGURE 5. Bubble motion with (a) $\theta = 60^\circ$, $\Delta t = 0.005$ (b) $\theta = 120.1^\circ$, $\Delta t = 0.001$

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