Review of recent advances in bulk-surface Cahn–Hilliard systems with dynamic boundary conditions

Kei Fong Lam

Department of Mathematics, Hong Kong Baptist University

1 Introduction

In recent years the Cahn–Hilliard equation [4] has drawn the attention of a large number of studies. Departing from its origin as a model for phase separation and demixing processes in binary alloys, later works have applied some variant of the Cahn–Hilliard equation in fluid flow [14], life sciences [2, 5, 11] and image processing [3, 22]. These usually affix the Cahn–Hilliard equation with a source term to enable the appropriate phenomena to be captured, but the fundamental behavior of the Cahn–Hilliard component remains unchanged. However, a new type of extensions in the form of dynamic boundary conditions offered potentially new dynamics not encountered in the aforementioned applications. The aim of this review is to provide a short overview of the recent developments surrounding some specific Cahn–Hilliard systems with dynamic boundary conditions.

2 Bulk-surface Cahn–Hilliard systems

Let Ω be a bounded domain with boundary $\Gamma := \partial\Omega$. For $T > 0$ we set $Q := \Omega \times (0, T)$ and $\Sigma := \Gamma \times (0, T)$. The standard Cahn–Hilliard equation takes the form

$$\partial_t u = \Delta\mu \qquad \text{in } Q, \tag{2.1a}$$

$$\mu = -\varepsilon\Delta u + \frac{1}{\varepsilon}F'(u) \text{ in } Q, \tag{2.1b}$$

$$u(t = 0) = u_0 \qquad \text{in } \Omega, \tag{2.1c}$$

where u is the phase field variable, μ is the associated chemical potential, F is a double well potential with derivative F' and $\varepsilon > 0$ is a small parameter. Standard choice for F is the quartic double well function $F(s) = (s^2 - 1)^2$ with two equal minima at $s = \pm 1$. The typical boundary conditions assigned are homogeneous Neumann conditions

$$\nabla u \cdot \boldsymbol{n} = \partial_{\boldsymbol{n}} u = 0, \quad \nabla\mu \cdot \boldsymbol{n} = 0 \quad \text{on } \Sigma,$$

where $\boldsymbol{n}$ is the outward unit normal on Γ. These boundary conditions enable the conservation of mass:

$$\frac{d}{dt}\int_\Omega u\,dx = 0 \quad \implies \quad \int_\Omega u(t)\,dx = \int_\Omega u_0\,dx$$

for all $t > 0$, which comes from integrating (2.1a) and applying $\partial_{\boldsymbol{n}}\mu = 0$, while $\partial_{\boldsymbol{n}} u = 0$ provides a static 90 degree contact angle for the *sharp* interface that separate the bulk regions $\{u = 1\}$ and $\{u = -1\}$ with the external boundary $\partial\Omega$, see e.g. [1].

While the Cahn–Hilliard equation with homogeneous Neumann conditions has been well-studied in the literature, see e.g. [19, 21] and the references cited therein, the model itself neglects

further interactions with the domain boundary. This limits applications in which interactions between domain boundary and domain interior play a significant role. One prominent example is that of the moving contact line problem [20].

A first approach towards proposing dynamic boundary conditions for the Cahn–Hilliard equation is to look at the associated energy functional. We recall the Ginzburg–Landau functional

$$E_\Omega(u) = \int_\Omega \frac{\varepsilon}{2}|\nabla u|^2 + \frac{1}{\varepsilon}F(u)\,dx$$

in which the Cahn–Hilliard equation (2.1) can be interpreted as the H^{-1}-gradient flow of E_Ω. We now add a surface energy functional

$$E_\Gamma(u) = \int_\Gamma \frac{\kappa\delta}{2}|\nabla_\Gamma u|^2 + \frac{1}{\delta}G(u)\,dS.$$

Here, ∇_Γ denotes the surface gradient on Γ, G is a surface potential, $\kappa \geq 0$ and $\delta > 0$ are constants. Denoting by $E = E_\Omega + E_\Gamma$ the total energy functional, let us highlight two Cahn–Hilliard models with dynamic boundary conditions that have been widely studied.

2.1   Goldstein–Miranville–Schimperna (GMS) model

The first prominent bulk-surface Cahn–Hilliard (BSCH) system to be mentioned is the one proposed by Goldstein, Miranville and Schimperna [13], which reads as follows:

$$\partial_t u = \Delta\mu, \qquad \mu = -\varepsilon\Delta u + \frac{1}{\varepsilon}F'(u) \qquad\qquad \text{in } Q, \qquad (2.2a)$$

$$\partial_t u = \Delta_\Gamma\theta - \beta\partial_{\boldsymbol{n}}\mu, \quad \theta = -\kappa\delta\Delta_\Gamma u + \frac{1}{\delta}G'(u) + \varepsilon\partial_{\boldsymbol{n}}u \text{ on } \Sigma, \qquad (2.2b)$$

$$\mu|_\Sigma = \beta\theta \qquad\qquad\qquad \text{on } \Sigma. \qquad (2.2c)$$

In the above, Δ_Γ denotes the surface Laplacian and θ is the surface chemical potential. The bulk chemical potential μ and the surface chemical potential θ are linked by the third equation, where we see that these two quantities can differ by the factor β. This GMS model can be regarded as an extension of a previous model introduced by Gal [6]. An important property of the GMS model is the mass conservation law

$$\beta\int_\Omega u(t)\,dx + \int_\Gamma u(t)\,dS = \beta\int_\Omega u(0)\,dx + \int_\Gamma u(0)\,dS, \qquad (2.3)$$

and sufficiently regular solutions satisfy the energy dissipation law

$$\frac{d}{dt}E(u) + \int_\Omega |\nabla\mu|^2\,dx + \int_\Gamma |\nabla_\Gamma\theta|^2\,dS = 0.$$

2.2   Liu–Wu (LW) model

The second prominent BSCH model to be mentioned is the one proposed by Liu and Wu [10, 17], which reads as follows:

$$\partial_t u = \Delta\mu, \quad \mu = -\varepsilon\Delta u + \frac{1}{\varepsilon}F'(u) \qquad\qquad \text{in } Q, \qquad (2.4a)$$

$$\partial_t u = \Delta_\Gamma\theta, \quad \theta = -\kappa\delta\Delta_\Gamma u + \frac{1}{\delta}G'(u) + \varepsilon\partial_{\boldsymbol{n}}u \text{ on } \Sigma, \qquad (2.4b)$$

$$\partial_{\boldsymbol{n}}\mu = 0 \qquad\qquad\qquad \text{on } \Sigma. \qquad (2.4c)$$

Again, θ is the surface chemical potential, but the most significant difference between the LW model and GMS model is the no-flux boundary condition $\partial_{\boldsymbol{n}}\mu = 0$ of the former. The effect of this is the decoupling of the bulk chemical potential μ and the surface chemical potential θ. Moreover, the mass conservation laws become decoupled as well:

$$\int_\Omega u(t)\,dx = \int_\Omega u(0)\,dx \quad \text{and} \quad \int_\Gamma u(t)\,dS = \int_\Gamma u(0)\,dS.$$

However, despite this significant departure from the GMS model, the LW model exhibit the same energy dissipation law:

$$\frac{d}{dt}E(u) + \int_\Omega |\nabla\mu|^2\,dx + \int_\Gamma |\nabla_\Gamma\theta|^2\,dS = 0.$$

2.3   Knopf–Lam–Liu–Metzger (KLLM) interpolation model

Both the GMS and LW models have attracted a significant amount of interests due to their contrasting mass conservation properties but sharing the same energy dissipation law. A new model was proposed by Knopf, Lam, Liu and Metzger in [15] that serve to connect the LW and GMS models. The KLLM model reads as

$$\partial_t u = \Delta\mu, \qquad \mu = -\varepsilon\Delta u + \frac{1}{\varepsilon}F'(u) \qquad \text{in } Q, \qquad (2.5\text{a})$$

$$\partial_t u = \Delta_\Gamma\theta - \beta\partial_{\boldsymbol{n}}\mu, \quad \theta = -\kappa\delta\Delta_\Gamma u + \frac{1}{\delta}G'(u) + \varepsilon\partial_{\boldsymbol{n}}u \text{ on } \Sigma, \qquad (2.5\text{b})$$

$$L\partial_{\boldsymbol{n}}\mu = \beta\theta - \mu|_\Sigma \qquad \text{on } \Sigma. \qquad (2.5\text{c})$$

The KLLM model resembles the GMS model due to the appearance of $\beta\partial_{\boldsymbol{n}}\mu$ in the second equation, but differs in the relation between the bulk and surface chemical potentials. Namely, a Robin type boundary condition is postulated with a relaxation parameter $L > 0$. Notice that the mass conservation law for the KLLM model is exactly the same as the GMS model:

$$\beta\int_\Omega u(t)\,dx + \int_\Gamma u(t)\,dS = \beta\int_\Omega u(0)\,dx + \int_\Gamma u(0)\,dS,$$

but due to the Robin boundary condition the energy dissipation law differs by an additional contribution:

$$\frac{d}{dt}E(u) + \int_\Omega |\nabla\mu|^2\,dx + \int_\Gamma |\nabla_\Gamma\theta|^2\,dS + \int_\Gamma \frac{1}{L}(\beta\theta - \mu)^2\,dS = 0.$$

Despite their very different chemical and physical properties, the Robin boundary conditions allows us to obtain the LW and GMS models as appropriate asymptotic limits. It is clear that in the formal limit $L \to \infty$ one obtains

$$\partial_{\boldsymbol{n}}\mu = 0$$

which decouples the two chemical potential variables, leading to the LW model, while in the formal limit $L \to 0$ one obtains

$$\beta\theta = \mu,$$

which leads to the GMS model. Let us make these connections more rigorous with the following results, cf. [15, Thm. 4.1 and 4.2] for more details on the precise statements:

Theorem 2.1 (Asymptotic limit $L \to \infty$). *For $L > 0$, let (u^L, μ^L, θ^L) denote the unique weak solution to (2.5), then there exist functions (u^*, μ^*, θ^*) such that as $L \to \infty$,*

$$u^L \to u^* \text{ weakly* in } L^\infty(0,T;H^1(\Omega)) \cap H^1(0,T;H^1(\Omega)^*),$$

$$u^L|_\Sigma \to u^*|_\Sigma \text{ weakly* in } L^\infty(0,T;L^2(\Gamma)) \cap H^1(0,T;H^1(\Gamma)^*),$$

$$\mu^L \to \mu^* \text{ weakly in } L^2(0,T;H^1(\Omega)),$$

$$\theta^L \to \theta^* \text{ weakly in } L^2(0,T;H^1(\Gamma)),$$

$$\frac{1}{L}(\beta\theta^L - \mu^L|_\Sigma) \to 0 \text{ strongly in } L^2(\Sigma),$$

and (u^*, μ^*, θ^*) is the unique weak solution to the LW model. Furthermore, for $\kappa > 0$ there exists a positive constant C independent of L such that

$$\|\nabla(u^L - u^*)\|_{L^2(Q)} + \|\nabla_\Gamma(u^L - u^*)\|_{L^2(\Sigma)} \leq \frac{C}{\sqrt{L}},$$

$$\|\partial_{\boldsymbol{n}}\mu^L\|_{L^2(\Sigma)} \leq \frac{C}{\sqrt{L}},$$

$$\|u^L - u^*\|_{L^\infty(0,T;L^2)} + \|u^L - u^*\|_{L^\infty(0,T;L^2(\Gamma))} \leq \frac{C}{L^{1/4}}.$$

Theorem 2.2 (Asymptotic limit $L \to 0$). *For $L > 0$, let (u^L, μ^L, θ^L) denote the unique weak solution to (2.5), then there exist functions (u_*, μ_*, θ_*) such that as $L \to 0$,*

$$u^L \to u_* \text{ weakly* in } L^\infty(0,T;H^1(\Omega)) \cap H^1(0,T;H^1(\Omega)^*),$$

$$u^L|_\Sigma \to u_*|_\Sigma \text{ weakly* in } L^\infty(0,T;L^2(\Gamma)) \cap H^1(0,T;H^1(\Gamma)^*),$$

$$\mu^L \to \mu_* \text{ weakly in } L^2(0,T;H^1(\Omega)),$$

$$\theta^L \to \theta_* \text{ weakly in } L^2(0,T;H^1(\Gamma)),$$

$$\beta\theta^L - \mu^L|_\Sigma \to 0 \text{ strongly in } L^2(\Sigma),$$

and (u_*, μ_*, θ_*) is the unique weak solution to the GMS model. Furthermore, for $\kappa > 0$ there exists a positive constant C independent of L such that

$$\|\nabla(u^L - u_*)\|_{L^2(Q)} + \|\nabla_\Gamma(u^L - u_*)\|_{L^2(\Sigma)} \leq C\sqrt{L},$$

$$\|\beta\theta^L - \mu^L\|_{L^2(\Sigma)} \leq C\sqrt{L},$$

$$\|u^L - u_*\|_{L^\infty(0,T;L^2)} + \|u^L - u_*\|_{L^\infty(0,T;L^2(\Gamma))} \leq CL^{1/4}.$$

Through numerical simulations of the KLLM model performed for a setting involving a half-elliptical shaped droplet in contact with one side of a square domain $\Omega = (0,1)^2$, let us briefly describe the difference between the solution behavior for the LW, KLLM and GMS models:

- For the case $L = \infty$ i.e., the LW model, since the bulk and surface masses are conserved separately, the contact area of the droplet with the domain boundary did not change during the evolution. However, the elliptical droplet still tries to attain a circular shape with constant mean curvature, leading to an increasing of the contact angle.

- For the case $L = 0$, i.e., the GMS model and also for $L < \infty$, i.e., the KLLM model, since the weighted sum of the bulk and surface masses are conserved together, it permits the droplet contact area with the domain boundary to grow at the expense of reducing the size of the droplet in the interior. In particular we observe a spreading effect where the contact angle of the droplet decreases.

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- It has been observed that the contact area and contact angle of the droplet varies proportionally to the value of L. As L decreases the zero, the droplet contact area enlarges and the droplet contact angle decreases.

3   Recent extensions

In the study of moving contact lines for binary fluids, it is common to affix the Navier–Stokes equations with a Cahn–Hilliard equation with dynamic boundary conditions, see e.g. [7] for the case of matched densities and [8] for the case of unmatched densities. Leet us briefly outline the equations for the matched densities case, which now involves in addition to the phase field variable u and chemical potential μ, the fluid velocity $\boldsymbol{v}$ and the pressure p:

$$\mathrm{div}\,\boldsymbol{v} = 0 \qquad\qquad\qquad\qquad \text{in } Q, \tag{3.1a}$$

$$\partial_t \boldsymbol{v} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v} - \mathrm{div}(2\eta(u)D\boldsymbol{v}) + \nabla p = \mu\nabla u \qquad \text{in } Q, \tag{3.1b}$$

$$\partial_t u + \boldsymbol{v} \cdot \nabla u = \Delta\mu \qquad\qquad\qquad \text{in } Q, \tag{3.1c}$$

$$\mu = -\varepsilon\Delta u + \frac{1}{\varepsilon}F'(u) \qquad\qquad\qquad \text{in } Q, \tag{3.1d}$$

$$\boldsymbol{v} \cdot \boldsymbol{n} = 0, \quad \partial_{\boldsymbol{n}}\mu = 0 \qquad\qquad\qquad \text{on } \Sigma, \tag{3.1e}$$

$$\partial_t u + \boldsymbol{v}_\tau \cdot \nabla_\Gamma u = -\partial_{\boldsymbol{n}} u + \Delta_\Gamma u - G'(u) =: -\mathcal{L}(u) \text{ on } \Sigma, \tag{3.1f}$$

$$\boldsymbol{v}_\tau + (2\eta(u)D\boldsymbol{v} \cdot \boldsymbol{n})_\tau = \mathcal{L}(u)\nabla_\Gamma u \qquad\qquad \text{on } \Sigma. \tag{3.1g}$$

In the above model, $D\boldsymbol{v} = (\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^\top)/2$ is the symmetric strain tensor, η is the viscosity function, $\boldsymbol{v}_\tau$ is the tangential component of $\boldsymbol{v}$ on the boundary. Besides the appearance of a convection term in the Cahn–Hilliard equation, which couples it with the Navier–Stokes system, for the boundary condition it features a surface Allen–Cahn type equation for u, which serves to capture the dynamics of the moving contact line separating the two fluids when touching the domain boundary.

In the recent work [12] the authors devised a new type of dynamic boundary condition for (3.1) that is of surface Cahn–Hilliard type. Instead of (3.1e)-(3.1g), it has been proposed to furnish with the following boundary conditions on Σ:

$$\boldsymbol{v} \cdot \boldsymbol{n} = 0, \tag{3.2a}$$

$$\partial_t u + \boldsymbol{v}_\tau \cdot \nabla_\Gamma u = \Delta_\Gamma \theta - \beta\partial_{\boldsymbol{n}}\mu, \tag{3.2b}$$

$$L\partial_{\boldsymbol{n}}\mu = \beta\theta - \mu, \tag{3.2c}$$

$$\boldsymbol{v}_\tau + (2\eta(u)D\boldsymbol{v} \cdot \boldsymbol{n})_\tau = (-u\nabla_\Gamma\theta)_\tau. \tag{3.2d}$$

We observe elements of the KLLM model in (3.2b) and (3.2c), while (3.2d) now features the surface gradient of the surface chemical potential θ instead. Based on the numerical studies of the KLLM model on the influence of the parameter L (and hence the type of boundary conditions) on the contact angle, it would interesting to see the full effects when coupling with fluid motion via the Navier–Stokes equations and the generalized Navier boundary conditions. For the mathematical analysis of this type of model, we refer to a collection of recent works [9, 16, 18].

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Department of Mathematics
Hong Kong Baptist University
Kowloon Tong
Hong Kong
E-mail address: akflam@hkbu.edu.hk