FINITE ELEMENT APPROXIMATION OF SOLUBLE SURFACTANT SPREADING ON A THIN FILM*

JOHN W. BARRETT†, ROBERT NÜRNBERG†, AND MARK R. E. WARNER†

Abstract. We consider a fully practical finite element approximation of the following system of nonlinear degenerate parabolic equations:

$$\begin{aligned}\frac{\partial u}{\partial t} + \frac{1}{2} \nabla \cdot (u^2 \nabla [\sigma(v)]) - \frac{1}{3} \nabla \cdot (u^3 \nabla w) &= 0, \\ w &= -c \Delta u - \delta u^{-\nu} + a u^{-3}, \\ \frac{\partial v}{\partial t} + \nabla \cdot (u v \nabla [\sigma(v)]) - \frac{1}{2} \nabla \cdot (u^2 v \nabla w) - \rho_s \Delta v - K(\psi - v) &= 0, \\ \frac{\partial \psi}{\partial t} + \frac{1}{2} u \nabla [\sigma(v)] \cdot \nabla \psi - \frac{1}{3} u^2 \nabla w \cdot \nabla \psi - \rho_b u^{-1} \nabla \cdot (u \nabla \psi) + \beta K u^{-1}(\psi - v) &= 0.\end{aligned}$$

The above equations model a Marangoni driven thin film laden with a soluble surfactant, in which the bulk surfactant concentration has been vertically averaged. The model accounts for the presence of both attractive, $a \geq 0$, and repulsive, $\delta > 0$ with $\nu > 3$, van der Waals forces. Here u is the height of the film, v is the concentration of the interfacial surfactant species, ψ is the concentration of the surfactant species within the bulk phase, and $\sigma(v) := 1 - v$ is the typical surface tension. Moreover, $\rho_s \geq 0$, $\rho_b > 0$, and $c > 0$ are the inverses of the surface Peclet number, the bulk Peclet number, and the modified capillary number, respectively; finally, $\beta > 0$ and $K > 0$ are parameters that characterize the solubility and the rate of interfacial adsorption. In addition to showing stability bounds for our approximation, we prove convergence and hence existence of a solution to this nonlinear degenerate parabolic system (i) in one space dimension when $\rho_s > 0$ and, moreover, (ii) in two space dimensions if, in addition, $\nu \geq 7$. Furthermore, iterative schemes for solving the resulting nonlinear discrete system are discussed. Finally, some numerical experiments are presented.

Key words. thin film flow, surfactant, fourth order degenerate parabolic system, finite elements, convergence analysis

AMS subject classifications. 65M60, 65M12, 35K55, 35K65, 35K35, 76A20, 76D08

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1. Introduction. In the recent papers [5, 6], abbreviated to BGN and BN throughout this paper, the authors proposed and analyzed a fully practical finite element approximation of a system of nonlinear degenerate parabolic equations describing an *insoluble* surfactant driven monolayer. Here, we generalize that system to a model in which the chemical may demonstrate varying degrees of solubility allowing for adsorption and desorption between the bulk phase and an interfacial concentration. This extended model is given by

$$(1.1a) \quad \frac{\partial u}{\partial t} + \frac{1}{2} \nabla \cdot (u^2 \nabla [\sigma(v)]) - \frac{1}{3} \nabla \cdot (u^3 \nabla w) = 0,$$

$$(1.1b) \quad w = -c \Delta u + \phi(u),$$

$$(1.1c) \quad \frac{\partial v}{\partial t} + \nabla \cdot (u v \nabla [\sigma(v)]) - \frac{1}{2} \nabla \cdot (u^2 v \nabla w) - \rho_s \Delta v - K(\psi - v) = 0,$$

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†Department of Mathematics, Imperial College, London, SW7 2AZ, UK (j.barrett@imperial.ac.uk, rn@imperial.ac.uk, m.r.warner@imperial.ac.uk). The third author was supported by EPSRC grant GR/S35660/01.

$$\begin{aligned}
 & \frac{\partial \psi}{\partial t} + \frac{1}{2} u \nabla [\sigma(v)] \cdot \nabla \psi - \frac{1}{3} u^2 \nabla w \cdot \nabla \psi - \rho_b u^{-1} \nabla \cdot (u \nabla \psi) \\
 (1.1d) \quad & + \beta K u^{-1} (\psi - v) = 0
 \end{aligned}$$

in Ω_T , where $\Omega_T := \Omega \times (0, T]$ and Ω is a bounded domain in $\mathbb{R}^d$, $d = 1$ or 2 . The above model, derived using lubrication theory and a cross-sectional averaging technique that removes the vertical dependence of the bulk species [12], models the flow of a surface tension gradient driven surfactant (chemical) laden thin film. Here u denotes the film height, v the concentration of the interfacial surfactant species, ψ the cross-sectionally averaged chemical concentration per unit height within the fluid layer, and w the pressure (reduced if van der Waals forces are present, that is, $\phi \neq 0$). In addition, $\sigma \in C^1(\mathbb{R}_{\geq 0})$ with

$$(1.2) \quad \sigma(s) \geq 0, \quad \sigma'(s) < 0 \quad \forall s \in \mathbb{R}_{\geq 0}$$

is the constitutive equation of state relating the surface tension σ to the interfacial concentration v . We note that σ is a strictly monotonically decreasing function of v , which is natural to assume as the surfactant lowers surface tension. An empirical model proposed by Sheludko [15], often used in the engineering literature and that maps $\sigma : [0, 1] \rightarrow [0, 1]$, is

$$(1.3) \quad \sigma(s) := (\alpha + 1) [1 + \theta(\alpha) s]^{-3} - \alpha, \quad \text{where } \theta(\alpha) := (1 + \alpha^{-1})^{\frac{1}{3}} - 1,$$

in which $\alpha \in \mathbb{R}_{>0}$ relates to the activity of the surfactant; cf. [11, p. 262]. Of course the above model assumes that $v(\cdot, \cdot) \in [0, 1]$, which is a physically reasonable assumption. In modeling studies it is often further assumed that the surfactant concentration is dilute, in which case the limit $\alpha \rightarrow \infty$ is taken, and the equation of state (1.3) simplifies to $\sigma(s) := 1 - s$. For the van der Waals forces in (1.1b), we take the form suggested in [13]; that is,

$$(1.4) \quad \phi(u) = \phi^+(u) + \phi^-(u), \quad \phi^+(u) := -\delta u^{-\nu}, \quad \nu > 3, \quad \phi^-(u) := a u^{-3},$$

where $a \in \mathbb{R}_{\geq 0}$ is the scaled dimensionless Hamaker constant and $\delta \in \mathbb{R}_{\geq 0}$ represents the effect of repulsive van der Waals forces. In (1.1a)–(1.1d), $\rho_s \in \mathbb{R}_{\geq 0}$, $\rho_b \in \mathbb{R}_{>0}$, and $c \in \mathbb{R}_{>0}$ are a nondimensional surface diffusivity (inverse of the surface Peclet number), a bulk diffusivity (inverse of the bulk Peclet number), and the modified capillary number, respectively. In order to permit the cross-sectional averaging process one has assumed that vertical diffusion is sufficiently fast for the bulk concentration to become independent of y , the vertical variable, at leading order. A necessary condition of this process is that the product of ρ_b and the dimensional film aspect ratio squared must be negligible at leading order in the lubrication approximation, and hence in practical applications ρ_b is not “too large.” The parameter $\beta \in \mathbb{R}_{>0}$ indicates the degree of solubility of the chemical and emerges from the lubrication scaling as a ratio of the rate of adsorption to the rate of desorption of the chemical at the interface, $y = u$. We note that in the insoluble limit, $\beta \rightarrow \infty$, whereby the chemical accumulates preferentially at the interface, (1.1d) collapses to $\psi = v$, and the system (1.1a)–(1.1d) reduces to the insoluble surfactant system, (1.1a)–(1.1c) with $\psi \equiv v$, considered in BGN and BN. Finally, $K \in \mathbb{R}_{>0}$ is a parameter that describes the ratio of the time scale of the flow to the time scale of desorption. Applications of the system (1.1a)–(1.1d) range from the medical treatment of premature infants to industrial coating and drying processes; see BGN for further details and references.

As u and v can take on zero values, (1.1a)–(1.1d) is a degenerate parabolic system, which is fourth order in u . This degeneracy makes the analysis/numerical analysis of the system particularly difficult. As there is no maximum principle for parabolic equations of fourth order, a naive discretization does not guarantee the nonnegativity of the approximation to u . If $\delta = 0$, following [2], BGN imposed the nonnegativity of the discrete approximation to u as a constraint; whereas if $\delta > 0$, the positivity of the approximation to u can be guaranteed for an appropriate discretization through the singularity in ϕ^+ . In both cases, BGN proposed a finite element approximation of the insoluble surfactant system, (1.1a)–(1.1c) with $\psi \equiv v$, and were able to derive stability bounds in space dimensions $d = 1$ and 2 . However, their main convergence result was restricted to $\rho_s > 0$ and one space dimension. The latter was due to the fact that the a priori bounds they derived guarantee only in one space dimension that the discrete approximation to u is uniformly bounded and equicontinuous, which was necessary to be able to pass to the limit in the discrete problem. For similar reasons, the results on related degenerate parabolic equations of fourth order in [1, 2, 3, 4, 8, 10] were restricted to one space dimension. However, recently in [9], Grün proved convergence in two space dimensions of a finite element approximation to the thin film equation in the absence of surfactant/chemical, (1.1a)–(1.1b) with $v \equiv 0$ and $u(\cdot, 0) > 0$. In BN the techniques in BGN and [9] were adapted to propose a finite element approximation to the insoluble surfactant system, (1.1a)–(1.1c) with $\psi \equiv v$, and prove convergence in one space dimension if $\rho_s, a, \delta, u(\cdot, 0) > 0$ and, moreover, in two space dimensions if in addition $\nu \geq 7$. It is the aim of this paper to adapt the techniques in BN in order to prove convergence of a finite element approximation to (1.1a)–(1.1d). To this end, we will identify and exploit an underlying Lyapunov structure and extend the usage of two entropy-type estimates that were introduced in BGN and BN, respectively.

Throughout this paper, as in BGN and BN, we restrict ourselves to the linearized form of the constitutive equation of state

$$(1.5) \quad \sigma(v) := 1 - v,$$

the $\alpha \rightarrow \infty$ limit of (1.3). However, the techniques in this paper do apply to a general σ satisfying (1.2); see Remark 2.2 below. As remarked previously, the physically relevant values of v lie in the interval $[0, 1]$. Noting this, it is convenient for the analysis in this paper, as well as in BGN and BN, to replace the terms $u^i v$, $i = 1 \rightarrow 2$, in (1.1c) by $u^i \lambda(v)$, and similarly replace ψ in the first three terms of (1.1d) by $\lambda(\psi)$, where $\lambda : \mathbb{R} \rightarrow (-\infty, 1]$ is defined as

$$(1.6) \quad \lambda(s) := \min\{s, \lambda_M\}, \quad \text{with } \lambda_M := 1.$$

We will return to this point later in this section.

Altogether, in this paper we consider the following initial boundary value problem.

(P) Find functions $u, w, v, \psi : \Omega \times [0, T] \rightarrow \mathbb{R}$ such that

$$(1.7a) \quad \frac{\partial u}{\partial t} + \frac{1}{2} \nabla \cdot (u^2 \nabla [\sigma(v)]) - \frac{1}{3} \nabla \cdot (u^3 \nabla w) = 0 \quad \text{in } \Omega_T,$$

$$(1.7b) \quad w = -c \Delta u + \phi(u) \quad \text{in } \Omega_T,$$

$$(1.7c) \quad \begin{aligned} & \frac{\partial v}{\partial t} + \nabla \cdot (u \lambda(v) \nabla [\sigma(v)]) - \frac{1}{2} \nabla \cdot (u^2 \lambda(v) \nabla w) \\ & - \rho_s \Delta v - K(\psi - v) = 0 \end{aligned} \quad \text{in } \Omega_T,$$

$$\frac{\partial (u \lambda(\psi))}{\partial t} + \frac{1}{2} \nabla \cdot (u^2 \lambda(\psi) \nabla [\sigma(v)])$$

$$(1.7d) \quad -\frac{1}{3} \nabla \cdot (u^3 \lambda(\psi) \nabla w) - \rho_b \nabla \cdot (u \nabla \psi) + \beta K (\psi - v) = 0 \quad \text{in } \Omega_T,$$

$$(1.7e) \quad u(x, 0) = u^0(x) > 0, \quad v(x, 0) = v^0(x) \geq 0, \quad \psi(x, 0) = \psi^0(x) \geq 0 \quad \forall x \in \Omega,$$

$$(1.7f) \quad \begin{aligned} & \frac{1}{2} u^2 \frac{\partial[\sigma(v)]}{\partial \nu_{\partial\Omega}} - \frac{1}{3} u^3 \frac{\partial w}{\partial \nu_{\partial\Omega}} = \frac{\partial u}{\partial \nu_{\partial\Omega}} = u \lambda(v) \frac{\partial[\sigma(v)]}{\partial \nu_{\partial\Omega}} - \frac{1}{2} u^2 \lambda(v) \frac{\partial w}{\partial \nu_{\partial\Omega}} - \rho_s \frac{\partial v}{\partial \nu_{\partial\Omega}} \\ & = \frac{1}{2} u^2 \lambda(\psi) \frac{\partial[\sigma(v)]}{\partial \nu_{\partial\Omega}} - \frac{1}{3} u^3 \lambda(\psi) \frac{\partial w}{\partial \nu_{\partial\Omega}} - \rho_b u \frac{\partial \psi}{\partial \nu_{\partial\Omega}} = 0 \quad \text{on } \partial\Omega \times (0, T), \end{aligned}$$

where $\nu_{\partial\Omega}$ is normal to $\partial\Omega$, the Lipschitz boundary of Ω , and $T > 0$ is a fixed positive time. In the above $c, \rho_b, K, \beta \in \mathbb{R}_{>0}$, and $\rho_s \in \mathbb{R}_{\geq 0}$ are given constants, while $\sigma \in C^1(\mathbb{R}_{\geq 0})$ and $\phi : \mathbb{R}_{>0} \rightarrow \mathbb{R}$ are given by (1.2) and (1.4), with $a \geq 0$, $\delta > 0$, and u^0, v^0 , and ψ^0 are given initial profiles.

Note that (1.7d) is just a combination of (1.1a) and the modified (1.1d), obtained by multiplying (1.1a) with $\lambda(\psi)$ and the modified (1.1d) with u . This is crucial for the analysis in this paper, as it allows us to exploit a Lyapunov structure that was not available before. The other main ingredients of our approach are two energy estimates for the surfactant driven flow combined with a regularization procedure. In particular, for any given $\varepsilon \in (0, \lambda_M)$, we introduce the regularized function

$$(1.8) \quad \lambda_\varepsilon(s) := \max\{\lambda(s), \varepsilon\},$$

which yields the regularized system (P_ε) , i.e., (P) with $\{u, w, v, \psi, \lambda\}$ replaced by $\{u_\varepsilon, w_\varepsilon, v_\varepsilon, \psi_\varepsilon, \lambda_\varepsilon\}$. On defining the horizontal velocity field $\vec{V}_\varepsilon(y)$, similarly to BGN and BN, as

$$(1.9) \quad \vec{V}_\varepsilon(y) = y \nabla[\sigma(v_\varepsilon)] + \left(\frac{1}{2} y^2 - y u_\varepsilon\right) \nabla w_\varepsilon,$$

where the modified pressure $w_\varepsilon = -c \Delta u_\varepsilon + \phi(u_\varepsilon)$, we can recast the system (P_ε) in terms of this velocity field as follows:

$$(1.10a) \quad \frac{\partial u_\varepsilon}{\partial t} + \nabla \cdot \left(\int_0^{u_\varepsilon} \vec{V}_\varepsilon(y) dy \right) = 0,$$

$$(1.10b) \quad \frac{\partial v_\varepsilon}{\partial t} + \nabla \cdot (\lambda_\varepsilon(v_\varepsilon) \vec{V}_\varepsilon(u_\varepsilon)) = \rho_s \Delta v_\varepsilon + K (\psi_\varepsilon - v_\varepsilon),$$

$$(1.10c) \quad \frac{\partial(u_\varepsilon \lambda_\varepsilon(\psi_\varepsilon))}{\partial t} + \nabla \cdot \left(\lambda_\varepsilon(\psi_\varepsilon) \int_0^{u_\varepsilon} \vec{V}_\varepsilon(y) dy \right) = \rho_b \nabla \cdot (u_\varepsilon \nabla \psi_\varepsilon) - \beta K (\psi_\varepsilon - v_\varepsilon),$$

$$(1.10d) \quad \begin{aligned} & \nu_{\partial\Omega} \cdot \int_0^{u_\varepsilon} \vec{V}_\varepsilon(y) dy = \nu_{\partial\Omega} \cdot (\lambda_\varepsilon(v_\varepsilon) \vec{V}_\varepsilon(u_\varepsilon) - \rho_s \nabla v_\varepsilon) \\ & = \nu_{\partial\Omega} \cdot \left(\lambda_\varepsilon(\psi_\varepsilon) \int_0^{u_\varepsilon} \vec{V}_\varepsilon(y) dy - \rho_b u_\varepsilon \nabla \psi_\varepsilon \right) = 0. \end{aligned}$$

We see from (1.9) that (P) is derived on assuming a no-slip condition at $y = 0$.

In order to derive the crucial energy estimates, we introduce the regularized function F_ε such that

$$(1.11) \quad F_\varepsilon''(s) = [\lambda_\varepsilon(s)]^{-1} \quad \text{and} \quad F_\varepsilon(1) = F_\varepsilon'(1) = 0,$$

which implies that

$$(1.12) \quad F_\varepsilon(s) := \begin{cases} \frac{s^2 - \varepsilon^2}{2\varepsilon} + (\ln \varepsilon - 1)s + 1, & s \leq \varepsilon, \\ s(\ln s - 1) + 1, & \varepsilon \leq s \leq 1, \\ \frac{1}{2}(s - 1)^2, & 1 \leq s. \end{cases}$$

Hence $F_\varepsilon \in C^{2,1}(\mathbb{R})$ and, for later purposes, we note that

$$(1.13) \quad F_\varepsilon(s) \geq \frac{s^2}{4} - \frac{1}{2} \quad \forall s \geq 0 \quad \text{and} \quad F_\varepsilon(s) \geq \frac{s^2}{2\varepsilon} \quad \forall s \leq 0;$$

see (2.4) in BGN. In addition, it is easily deduced that

$$(1.14) \quad \frac{[F_\varepsilon'(s)]^2}{F_\varepsilon''(s)} \leq \begin{cases} 2\varepsilon^{-1}[s]_-^2 + 8 \exp(-1), & s \leq \varepsilon, \\ 4 \exp(-2), & \varepsilon \leq s \leq 1, \end{cases} \quad \text{where } [s]_\pm := \pm \max\{\pm s, 0\}.$$

We also introduce

$$(1.15) \quad \widehat{F}_\varepsilon(s) := F_\varepsilon(\lambda_\varepsilon(s)) \equiv \lambda_\varepsilon(s) F_\varepsilon'(s) - s + 1.$$

As F_ε is convex, it follows that

$$(1.16) \quad [\lambda_\varepsilon(s) - \lambda_\varepsilon(r)] F_\varepsilon'(s) \geq \widehat{F}_\varepsilon(s) - \widehat{F}_\varepsilon(r) \quad \forall r, s \in \mathbb{R}.$$

We will now derive several formal estimates for $\{u_\varepsilon, w_\varepsilon, v_\varepsilon, \psi_\varepsilon\}$. Testing equation (1.10a) with w_ε and combining and noting (1.9) and (1.10d) yields that

$$(1.17) \quad \frac{d}{dt} \int_\Omega \left[\frac{c}{2} |\nabla u_\varepsilon|^2 + \Phi(u_\varepsilon) \right] dx + \int_\Omega \left(\int_0^{u_\varepsilon} |\partial_y \vec{\mathcal{V}}_\varepsilon(y)|^2 dy \right) dx = - \int_\Omega \vec{\mathcal{V}}_\varepsilon(u_\varepsilon) \cdot \nabla v_\varepsilon dx,$$

where Φ is an antiderivative of ϕ , i.e., $\Phi' \equiv \phi$. Testing (1.10b) with $F_\varepsilon'(v_\varepsilon)$ and noting (1.10d) and (1.11) yields that

$$(1.18) \quad \begin{aligned} & \frac{d}{dt} \int_\Omega F_\varepsilon(v_\varepsilon) dx + \rho_s \int_\Omega F_\varepsilon''(v_\varepsilon) |\nabla v_\varepsilon|^2 dx \\ &= \int_\Omega \vec{\mathcal{V}}_\varepsilon(u_\varepsilon) \cdot \nabla v_\varepsilon dx + K \int_\Omega (\psi_\varepsilon - v_\varepsilon) F_\varepsilon'(v_\varepsilon) dx. \end{aligned}$$

Moreover, it follows from testing (1.10c) with $F_\varepsilon'(\psi_\varepsilon)$ and testing (1.10a) with $\psi_\varepsilon - 1$, on noting (1.15), $F_\varepsilon'(\lambda_\varepsilon(\psi_\varepsilon)) \frac{\partial[\lambda_\varepsilon(\psi_\varepsilon)]}{\partial t} = F_\varepsilon'(\psi_\varepsilon) \frac{\partial[\lambda_\varepsilon(\psi_\varepsilon)]}{\partial t}$, (1.10d), and (1.11), that

$$(1.19) \quad \begin{aligned} & \frac{d}{dt} \int_\Omega u_\varepsilon \widehat{F}_\varepsilon(\psi_\varepsilon) dx = \int_\Omega \frac{\partial(u_\varepsilon \lambda_\varepsilon(\psi_\varepsilon))}{\partial t} F_\varepsilon'(\psi_\varepsilon) dx - \int_\Omega \frac{\partial u_\varepsilon}{\partial t} (\psi_\varepsilon - 1) dx \\ &= -\rho_b \int_\Omega u_\varepsilon F_\varepsilon''(\psi_\varepsilon) |\nabla \psi_\varepsilon|^2 dx - \beta K \int_\Omega (\psi_\varepsilon - v_\varepsilon) F_\varepsilon'(\psi_\varepsilon) dx. \end{aligned}$$

Combining (1.17), (1.18), and (1.19) yields that

$$\begin{aligned}
 & \frac{d}{dt} \int_{\Omega} \left[\frac{c}{2} |\nabla u_{\varepsilon}|^2 + \Phi(u_{\varepsilon}) + F_{\varepsilon}(v_{\varepsilon}) + \frac{1}{\beta} u_{\varepsilon} \widehat{F}_{\varepsilon}(\psi_{\varepsilon}) \right] dx + \rho_s \int_{\Omega} F_{\varepsilon}''(v_{\varepsilon}) |\nabla v_{\varepsilon}|^2 dx \\
 & + \frac{\rho_b}{\beta} \int_{\Omega} u_{\varepsilon} F_{\varepsilon}''(\psi_{\varepsilon}) |\nabla \psi_{\varepsilon}|^2 dx + \int_{\Omega} \left(\int_0^{u_{\varepsilon}} |\partial_y \vec{\mathcal{V}}_{\varepsilon}(y)|^2 dy \right) dx \\
 & + K \int_{\Omega} (F'_{\varepsilon}(\psi_{\varepsilon}) - F'_{\varepsilon}(v_{\varepsilon})) (\psi_{\varepsilon} - v_{\varepsilon}) dx = 0.
 \end{aligned}
 \tag{1.20}$$

Due to the singularity in Φ at the origin, it immediately follows from (1.20) that $u_{\varepsilon}(\cdot, t) > 0$ for all $t \in (0, T)$ if $u_{\varepsilon}(\cdot, 0) > 0$. In addition, it follows from (1.9), on applying a Young inequality

$$|rs| \leq \frac{\gamma}{2} r^2 + \frac{1}{2\gamma} s^2 \quad \forall r, s \in \mathbb{R}, \quad \gamma \in \mathbb{R}_{>0},
 \tag{1.21}$$

that

$$\int_0^{u_{\varepsilon}} |\partial_y \vec{\mathcal{V}}_{\varepsilon}(y)|^2 dy \geq \frac{1}{8} u_{\varepsilon} |\nabla[\sigma(v_{\varepsilon})]|^2 + \frac{1}{21} u_{\varepsilon}^3 |\nabla w_{\varepsilon}|^2;
 \tag{1.22}$$

see (1.7) in BGN for details.

From (1.20), (1.11), (1.8), and (1.6), one can deduce uniform bounds on ∇v_{ε} and $u_{\varepsilon} \nabla \psi_{\varepsilon}$ in $L^2(\Omega_T)$. We note the crucial role that the cut-off λ_M in (1.6) plays in these estimates. Of course the cut-off λ_M can be chosen arbitrarily large, and it played no real role in our finite element approximation of (P_{ε}) , as our computed approximations to both v_{ε} and ψ_{ε} were always strictly less than λ_M , which we set to be one. However, as it does not appear possible to obtain a priori $L^{\infty}(\Omega_T)$ bounds on v_{ε} and ψ_{ε} , one requires some (arbitrarily large) cut-off in (1.6) and hence in certain coefficients in (1.7a)–(1.7f), as the Lyapunov structure above is based on the relationship (1.11).

In order to obtain the second estimate, we also define a function $G \in C^{\infty}(\mathbb{R}_{>0})$ such that $u^3 \nabla[G'(u)] = \nabla u$; that is,

$$G''(s) = s^{-3} \Rightarrow G'(s) = -\frac{1}{2} s^{-2} \Rightarrow G(s) = \frac{1}{2} s^{-1},
 \tag{1.23}$$

where the constants of integration have been chosen to be zero. Testing (1.10a) with $G'(u_{\varepsilon})$ and testing (1.1b) with $-\Delta u_{\varepsilon}$ yields, on noting (1.10d) and applying (1.21) (see (1.10)–(1.12) in BN for details), that

$$\begin{aligned}
 & \frac{d}{dt} \int_{\Omega} G(u_{\varepsilon}) dx + \frac{c}{3} \int_{\Omega} |\Delta u_{\varepsilon}|^2 dx + \frac{1}{4} \int_{\Omega} (\phi^+)'(u_{\varepsilon}) |\nabla u_{\varepsilon}|^2 dx \\
 & \leq C \left[\int_{\Omega} u_{\varepsilon} |\nabla[\sigma(v_{\varepsilon})]|^2 dx + \int_{\Omega} |\nabla u_{\varepsilon}|^2 dx \right].
 \end{aligned}
 \tag{1.24}$$

From (1.24), (1.20), and (1.22) one can show that u_{ε} is uniformly bounded in $L^2(0, T; H^2(\Omega))$ if $u_{\varepsilon}(\cdot, 0) > 0$. Furthermore, the bound (1.13) together with (1.20) yields that $\int_{\Omega_T} [v_{\varepsilon}]_-^2 dx dt \leq C \varepsilon$. One can use this, together with the last bound in (1.20), to deduce that $\int_{\Omega_T} F_{\varepsilon}(\psi_{\varepsilon}) dx dt \leq C$ and hence that $\int_{\Omega_T} [\psi_{\varepsilon}]_-^2 dx dt \leq C \varepsilon$.

It is the goal of this paper to derive a finite element method that is consistent with the formal energy estimates (1.20) and (1.24). We stress that it is only the bound (1.24) that requires the presence of the repulsive van der Waals forces, $\delta > 0$, to control the surfactant term in (1.10a). In the absence of a surfactant/chemical, (1.24) holds with $(a, \delta > 0)$ and without $(a = \delta = 0)$ van der Waals forces.

This paper is organized as follows. In section 2 we formulate a fully practical finite element approximation of the degenerate system (P) and derive discrete analogues of the energy estimates (1.20) and (1.24). In doing so, we adapt a technique introduced in [17] and [10] for deriving a discrete entropy bound for the thin film equation. In section 3 we prove convergence, and hence existence, of a solution to the system (P) in one space dimension if $\rho_s, \delta > 0$ and in two space dimensions if, in addition, $\nu \geq 7$. In section 4 we state an iterative scheme for solving the nonlinear discrete system at each time level and present some numerical computations in both one and two space dimensions.

Finally we note that there is very little work in the PDE literature on surfactant-type problems. To our knowledge, there is no work on the degenerate soluble system (P). A numerical study of (P) can be found in [16]. We stress that this paper is a nontrivial extension of the insoluble surfactant system, (1.7a)–(1.7c) with $\psi = v$, studied in BN. First, one has to identify the Lyapunov structure for (P), which we have outlined in this introduction. Second, proving convergence of our finite element approximation to (P) and hence proving existence of a solution to (P) is far more difficult in this case. As stated earlier, we will establish a finite element approximation, which satisfies discrete analogues of (1.20) and (1.24). For the insoluble surfactant one has control on the discrete analogue of $\int_{\Omega_T} |\nabla v_\varepsilon|^2 dx dt$ if $\rho_s > 0$, whereas for the chemical we have control only on the discrete analogue of $\int_{\Omega_T} u_\varepsilon |\nabla \psi_\varepsilon|^2 dx dt$. This degeneracy, as we have no a priori positive lower bound on u_ε , causes a number of new difficulties in the convergence analysis.

Notation and auxiliary results. Let $D \subset \mathbb{R}^d$, $d = 1$ or 2 , with a Lipschitz boundary ∂D if $d = 2$. We adopt the standard notation for Sobolev spaces, denoting the norm of $W^{m,q}(D)$ ($m \in \mathbb{N}$, $q \in [1, \infty]$) by $\|\cdot\|_{m,q,D}$ and the seminorm by $|\cdot|_{m,q,D}$. We extend these norms and seminorms in the natural way to the corresponding spaces of vector and matrix valued functions. For $q = 2$, $W^{m,2}(D)$ will be denoted by $H^m(D)$ with the associated norm and seminorm written as, respectively, $\|\cdot\|_{m,D}$ and $|\cdot|_{m,D}$. For notational convenience, we drop the domain subscript on the above norms and seminorms in the case $D \equiv \Omega$. Throughout $(\cdot, \cdot)$ denotes the standard L^2 inner product over Ω , while q' denotes for any $q \in [1, \infty]$ the “dual exponent” such that $\frac{1}{q} + \frac{1}{q'} = 1$. In addition we define $f\eta := (\eta, 1)/\underline{m}(\Omega)$ for all $\eta \in L^1(\Omega)$, where $\underline{m}(D)$ denotes the measure of D .

It is convenient to introduce the operator $\mathcal{G} : (W^{1,q'}(\Omega))' \rightarrow W^{1,q}(\Omega)$ such that

$$(1.25) \quad (\nabla \mathcal{G}z, \nabla \eta) + (\mathcal{G}z, \eta) = \langle z, \eta \rangle_{q'} \quad \forall \eta \in W^{1,q'}(\Omega),$$

where here and throughout $\langle \cdot, \cdot \rangle_{q'}$ denotes the duality pairing between $(W^{1,q'}(\Omega))'$ and $W^{1,q'}(\Omega)$ for any $q \in (1, 2]$.

Throughout C denotes a generic constant independent of h , τ , and ε , the mesh and temporal discretization parameters and the regularization parameter. In addition, $C(a_1, \dots, a_I)$ denotes a constant depending on the arguments $\{a_i\}_{i=1}^I$. Furthermore, $\cdot^{(*)}$ denotes an expression with or without the superscript $\star$.

2. Finite element approximation. We consider the finite element approximation of (P) under the following assumptions on the mesh.

- (A) Let Ω be a convex polygonal domain if $d = 2$. Let $\{\mathcal{T}^h\}_{h>0}$ be a quasi-uniform family of partitionings of Ω into disjoint open simplices κ with $h_\kappa := \text{diam}(\kappa)$ and $h := \max_{\kappa \in \mathcal{T}^h} h_\kappa$, so that $\bar{\Omega} = \cup_{\kappa \in \mathcal{T}^h} \bar{\kappa}$. In addition, it is assumed for $d = 2$ that all simplices $\kappa \in \mathcal{T}^h$ are right-angled.

Associated with $\mathcal{T}^h$ is the finite element space $S^h := \{\chi \in C(\bar{\Omega}) : \chi|_\kappa \text{ is linear for all } \kappa \in \mathcal{T}^h\} \subset H^1(\Omega)$. We also introduce $S_{\geq 0}^h := \{\chi \in S^h : \chi \geq 0 \text{ in } \Omega\} \subset H_{\geq 0}^1(\Omega) := \{\eta \in H^1(\Omega) : \eta \geq 0 \text{ a.e. in } \Omega\}$ and similarly $S_{> 0}^h$ and $H_{> 0}^1(\Omega)$. Let J be the set of nodes of $\mathcal{T}^h$ and $\{p_j\}_{j \in J}$ the coordinates of these nodes. Let $\{\chi_j\}_{j \in J}$ be the standard basis functions for S^h ; that is, $\chi_j \in S_{\geq 0}^h$ and $\chi_j(p_i) = \delta_{ij}$ for all $i, j \in J$. We introduce $\pi^h : C(\bar{\Omega}) \rightarrow S^h$, the interpolation operator, such that $(\pi^h \eta)(p_j) = \eta(p_j)$ for all $j \in J$. A discrete semi-inner product on $C(\bar{\Omega})$ is then defined by

$$(2.1) \quad (\eta_1, \eta_2)^h := \int_{\Omega} \pi^h(\eta_1(x) \eta_2(x)) \, dx = \sum_{j \in J} m_j \eta_1(p_j) \eta_2(p_j),$$

where $m_j := (1, \chi_j) > 0$. The induced discrete seminorm is then $|\eta|_h := [(\eta, \eta)^h]^{\frac{1}{2}}$, where $\eta \in C(\bar{\Omega})$. We introduce also the L^2 projection $Q^h : L^2(\Omega) \rightarrow S^h$ defined by $(Q^h \eta, \chi)^h = (\eta, \chi)$ for all $\chi \in S^h$.

Similarly to the approach in [10, 17], we introduce matrices $\Lambda_\varepsilon : S^h \rightarrow [L^\infty(\Omega)]^{d \times d}$ and $\Xi : S_{> 0}^h \rightarrow [L^\infty(\Omega)]^{d \times d}$ such that for all $z^h \in S^h$, $\chi \in S_{> 0}^h$ and a.e. in Ω

$$(2.2a) \quad \Lambda_\varepsilon(z^h), \Xi(\chi) \text{ are symmetric and positive semidefinite,}$$

$$(2.2b) \quad \Lambda_\varepsilon(z^h) \nabla \pi^h[F'_\varepsilon(z^h)] = \nabla z^h, \quad [\Xi(\chi)]^3 \nabla \pi^h[G'(\chi)] = \nabla \chi.$$

The construction of these matrices can be found in BN. Throughout we make use of the fact that the matrices $\Xi(\chi)$ and $\Lambda_\varepsilon(z^h)$ commute for any $\chi \in S_{> 0}^h$ and $z^h \in S^h$.

As in BN, it is convenient to split Φ (recall (1.20)) into its convex and concave parts. We have for given $a \in \mathbb{R}_{\geq 0}$, $\delta \in \mathbb{R}_{> 0}$, and $\nu > 3$ that for all $s \in \mathbb{R}_{> 0}$

$$(2.3) \quad \Phi(s) = \Phi^+(s) + \Phi^-(s), \quad \text{where } \Phi^+(s) := \frac{\delta}{\nu-1} s^{1-\nu}, \quad \Phi^-(s) := -\frac{a}{2} s^{-2}.$$

It holds, on recalling (1.4), that $\phi^+ \equiv (\Phi^+)'$ and $\phi^- \equiv (\Phi^-)'$. For future reference, we note that the following hold for all $r, s \in \mathbb{R}_{> 0}$:

$$(2.4) \quad \begin{aligned} \Phi(s) &\geq -\frac{a(\nu-3)}{2(\nu-1)} \left(\frac{a}{\delta}\right)^{\frac{2}{\nu-3}} \quad \text{and} \\ -\Phi^-(s) &\leq \frac{a(\nu-3)}{2(\nu-1)} \left(\frac{2a}{\delta}\right)^{\frac{2}{\nu-3}} + \frac{1}{2} \Phi^+(s). \end{aligned}$$

In addition to $\mathcal{T}^h$, let $0 = t_0 < t_1 < \dots < t_{N-1} < t_N = T$ be a partitioning of $[0, T]$ into possibly variable time steps $\tau_n := t_n - t_{n-1}$, $n = 1 \rightarrow N$. We set $\tau := \max_{n=1 \rightarrow N} \tau_n$. For any given $\varepsilon \in (0, 1)$, we then consider the following fully practical finite element approximation of (P) with $\sigma(v)$ given by (1.5) and $\phi(u)$ given by (1.4):

$(P_\varepsilon^{h,\tau})$ For $n \geq 1$ find $\{U_\varepsilon^n, W_\varepsilon^n, V_\varepsilon^n, \Psi_\varepsilon^n\} \in [S^h]^4$ such that for all $\chi \in S^h$

$$(2.5a) \quad \left(\frac{U_\varepsilon^n - U_\varepsilon^{n-1}}{\tau_n}, \chi \right)^h + \frac{1}{3} ([\Xi(U_\varepsilon^n)]^3 \nabla W_\varepsilon^n, \nabla \chi) \\ = -\frac{1}{2} ([\Xi(U_\varepsilon^n)]^{\frac{3}{2}} [\Xi(U_\varepsilon^{n-1})]^{\frac{1}{2}} \nabla V_\varepsilon^{n-1}, \nabla \chi),$$

$$(2.5b) \quad c(\nabla U_\varepsilon^n, \nabla \chi) + (\phi^+(U_\varepsilon^n) + \phi^-(U_\varepsilon^{n-1}), \chi)^h = (W_\varepsilon^n, \chi)^h,$$

$$(2.5c) \quad \left(\frac{V_\varepsilon^n - V_\varepsilon^{n-1}}{\tau_n}, \chi \right)^h + \rho_s (\nabla V_\varepsilon^n, \nabla \chi) + (\Xi(U_\varepsilon^n) \Lambda_\varepsilon(V_\varepsilon^n) \nabla V_\varepsilon^n, \nabla \chi) \\ - K(\Psi_\varepsilon^n - V_\varepsilon^n, \chi)^h = -\frac{1}{2} ([\Xi(U_\varepsilon^n)]^2 \Lambda_\varepsilon(V_\varepsilon^n) \nabla W_\varepsilon^n, \nabla \chi),$$

$$(2.5d) \quad \left(\frac{U_\varepsilon^n \lambda_\varepsilon(\Psi_\varepsilon^n) - U_\varepsilon^{n-1} \lambda_\varepsilon(\Psi_\varepsilon^{n-1})}{\tau_n}, \chi \right)^h + \rho_b (U_\varepsilon^n \nabla \Psi_\varepsilon^n, \nabla \chi) \\ + \frac{1}{3} ([\Xi(U_\varepsilon^n)]^3 \Lambda_\varepsilon(\Psi_\varepsilon^n) \nabla W_\varepsilon^n, \nabla \chi) + \beta K(\Psi_\varepsilon^n - V_\varepsilon^n, \chi)^h \\ = -\frac{1}{2} ([\Xi(U_\varepsilon^n)]^{\frac{3}{2}} [\Xi(U_\varepsilon^{n-1})]^{\frac{1}{2}} \Lambda_\varepsilon(\Psi_\varepsilon^n) \nabla V_\varepsilon^{n-1}, \nabla \chi),$$

where $U_\varepsilon^0 \in S_{>0}^h$, $V_\varepsilon^0 \in S^h$, and $\Psi_\varepsilon^0 \in S^h$ are approximations of u^0 , v^0 , and ψ^0 , respectively, e.g., $U_\varepsilon^0 \equiv \pi^h u^0$ or $Q^h u^0$ and similarly for V_ε^0 and Ψ_ε^0 .

Remark 2.1. $(P_\varepsilon^{h,\tau})$ is the natural extension of the approximation of the insoluble surfactant system studied in BN. In particular, on setting $\Psi_\varepsilon^n \equiv V_\varepsilon^n$, $n = 1 \rightarrow N$, equations (2.5a)–(2.5c) collapse to the approximation in BN. Note that we approximate u^2 by $[\Xi(U_\varepsilon^n)]^{\frac{3}{2}} [\Xi(U_\varepsilon^{n-1})]^{\frac{1}{2}}$ in (2.5d) in order for our discrete stability bounds, the analogues of (1.20) and (1.24), to hold. Furthermore, as $U_\varepsilon^0 > 0$, one can ensure that $\Xi(U_\varepsilon^{n-1})$ and $\phi^-(U_\varepsilon^{n-1})$ are well defined for $n \geq 1$; see Theorem 2.3 below.

Remark 2.2. The restriction of σ to the linear case (1.5) is not crucial for the analysis in this paper. However, this choice simplifies our considerations and is also more practical. Different choices of σ , e.g., (1.3), can be incorporated; see Remark 2.2 in BN for details.

Below we recall some well-known results concerning S^h for any $\kappa \in \mathcal{T}^h$, $\chi, z^h \in S^h$, $m \in \{0, 1\}$, $p \in [1, \infty]$, $s \in [2, \infty]$ if $d = 1$, and $s \in (2, \infty]$ if $d = 2$:

$$(2.6) \quad |\chi|_{m,r,\kappa} \leq C h_\kappa^{-d(\frac{1}{p}-\frac{1}{r})} |\chi|_{m,p,\kappa} \quad \text{for any } r \in [p, \infty],$$

$$(2.7) \quad \lim_{h \rightarrow 0} \|(I - \pi^h)\eta\|_{1,s} = 0 \quad \forall \eta \in W^{1,s}(\Omega),$$

$$(2.8) \quad |(I - \pi^h)\eta|_{m,s,\kappa} \leq C h_\kappa^{1-m} |\eta|_{1,s,\kappa} \quad \forall \eta \in W^{1,s}(\kappa),$$

$$(2.9) \quad \|\pi^h[\chi z^h]\|_{1,p} \leq C [|\chi z^h|_{0,p} + |\chi \nabla z^h|_{0,p} + |z^h \nabla \chi|_{0,p}],$$

$$(2.10) \quad \int_\kappa \chi^2 dx \leq \int_\kappa \pi^h[\chi^2] dx \leq (d+2) \int_\kappa \chi^2 dx,$$

$$(2.11) \quad |(\chi, z^h) - (\chi, z^h)^h| \leq |(I - \pi^h)(\chi z^h)|_{0,1} \leq C h^{1+m} |\chi|_{m,p} |z^h|_{1,p'}.$$

On recalling (2.1), we see that the operator Q^h satisfies

$$(2.12) \quad (Q^h \eta)(p_j) = m_j^{-1}(\eta, \chi_j) \quad \forall j \in J \Rightarrow |Q^h \eta|_{0,\infty} \leq |\eta|_{0,\infty}, \quad \forall \eta \in L^\infty(\Omega),$$

and, in addition, it holds for $m \in \{0, 1\}$ that

$$(2.13) \quad |(I - Q^h)\eta|_{m,r} \leq C h^{1-m} |\eta|_{1,r} \quad \forall \eta \in W^{1,r}(\Omega), \quad \text{for any } r \in [2, \infty].$$

We note that assumption (A) and (1.11) yield that

$$(2.14) \quad \int_{\kappa} \nabla z^h \cdot \nabla \pi^h [F'_\varepsilon(z^h)] \, dx \geq |z^h|_{1,\kappa}^2 \quad \forall z^h \in S^h, \quad \forall \kappa \in \mathcal{T}^h;$$

see (2.13) in BN for details. It is also easily established that

$$(2.15) \quad |z^h|_{0,q} \leq C h^{-1} \|\mathcal{G} z^h\|_{1,q} \quad \forall z^h \in S^h, \quad \text{for any } q \in (1, 2].$$

We note that the results (2.13) and (2.15) above exploit the fact that we have a quasi-uniform family of partitionings $\{\mathcal{T}^h\}_{h>0}$. Finally, we introduce the “discrete Laplacian” operator $\Delta^h : S^h \rightarrow S^h$ such that $(\Delta^h z^h, \chi)^h = -(\nabla z^h, \nabla \chi)$ for all $\chi \in S^h$.

THEOREM 2.3. *Let $\phi(\cdot)$ satisfy (1.4) with $\delta > 0$. Let the assumptions (A) hold and $\{U_\varepsilon^{n-1}, V_\varepsilon^{n-1}, \Psi_\varepsilon^{n-1}\} \in S_{>0}^h \times [S^h]^2$. Then for all $\varepsilon \in (0, 1)$ and for all $h, \tau_n > 0$ there exists a solution $\{U_\varepsilon^n, W_\varepsilon^n, V_\varepsilon^n, \Psi_\varepsilon^n\} \in S_{>0}^h \times [S^h]^3$ to the n th step of $(P_\varepsilon^{h,\tau})$ with $f U_\varepsilon^n = f U_\varepsilon^{n-1}$ and $f(V_\varepsilon^n + \frac{1}{\beta} \pi^h [U_\varepsilon^n \lambda_\varepsilon(\Psi_\varepsilon^n)]) = f(V_\varepsilon^{n-1} + \frac{1}{\beta} \pi^h [U_\varepsilon^{n-1} \lambda_\varepsilon(\Psi_\varepsilon^{n-1})])$.*

Proof. Existence of a solution $\{U_\varepsilon^n, W_\varepsilon^n\} \in S_{>0}^h \times S^h$ to (2.5a)–(2.5b) follows from Lemma 2.1 in BN. To prove the existence of $\{V_\varepsilon^n, \Psi_\varepsilon^n\}$ to (2.5c)–(2.5d) we will make use of the *Brouwer fixed point theorem* (see, e.g., [14, Theorem 9.36, p. 357]). This is a nontrivial extension of the existence proof for V_ε^n in Theorem 2.1 of BGN. Let $\mathcal{J} := \#J$ and let $g : \mathbb{R}^{2\mathcal{J}} \rightarrow \mathbb{R}^{2\mathcal{J}}$ be defined by

$$\begin{aligned} g_j(\underline{V}, \underline{\Psi}) &:= \frac{1}{\tau_n} (V, \chi_j)^h + \rho_s (\nabla V, \nabla \chi_j) + (\Xi(U_\varepsilon^n) \Lambda_\varepsilon(V) \nabla V, \nabla \chi_j) \\ &\quad - K (\Psi - V, \chi_j)^h + \frac{1}{2} ([\Xi(U_\varepsilon^n)]^2 \Lambda_\varepsilon(V) \nabla W_\varepsilon^n, \nabla \chi_j), \\ g_{j+\mathcal{J}}(\underline{V}, \underline{\Psi}) &:= \frac{1}{\beta} \left[\frac{1}{\tau_n} (U_\varepsilon^n \lambda_\varepsilon(\Psi), \chi_j)^h + \rho_b (U_\varepsilon^n \nabla \Psi, \nabla \chi_j) \right. \\ &\quad \left. + \frac{1}{3} ([\Xi(U_\varepsilon^n)]^3 \Lambda_\varepsilon(\Psi) \nabla W_\varepsilon^n, \nabla \chi_j) + \beta K (\Psi - V, \chi_j)^h \right. \\ &\quad \left. + \frac{1}{2} ([\Xi(U_\varepsilon^n)]^{\frac{3}{2}} [\Xi(U_\varepsilon^{n-1})]^{\frac{1}{2}} \Lambda_\varepsilon(\Psi) \nabla V_\varepsilon^{n-1}, \nabla \chi_j) \right] \quad \forall j \in J, \end{aligned}$$

where $V \equiv \sum_{j \in J} V_j \chi_j$, $\Psi \equiv \sum_{j \in J} \Psi_j \chi_j$, and $\{\underline{V}, \underline{\Psi}\} := (V_1, \dots, V_{\mathcal{J}}, \Psi_1, \dots, \Psi_{\mathcal{J}})^T \in \mathbb{R}^{2\mathcal{J}}$. Hence a solution $\{V_\varepsilon^n, \Psi_\varepsilon^n\}$ of (2.5c)–(2.5d) is such that for $j = 1 \rightarrow \mathcal{J}$

$$g_j(\underline{V}_\varepsilon^n, \underline{\Psi}_\varepsilon^n) = \frac{1}{\tau_n} (V_\varepsilon^{n-1}, \chi_j)^h, \quad g_{j+\mathcal{J}}(\underline{V}_\varepsilon^n, \underline{\Psi}_\varepsilon^n) = \frac{1}{\beta \tau_n} (U_\varepsilon^{n-1} \lambda_\varepsilon(\Psi_\varepsilon^{n-1}), \chi_j)^h.$$

On noting Lemma 2.1 in BGN we have that g is continuous, and hence it is sufficient to show that g is coercive. We have that for all $\{V, \Psi\} \in [S^h]^2$

$$\begin{aligned}
 \sum_{j \in J} (g_j(\underline{V}, \underline{\Psi}) V_j + g_{j+\mathcal{J}}(\underline{V}, \underline{\Psi}) \Psi_j) &= \frac{1}{\tau_n} |V|_h^2 + \rho_s |V|_1^2 \\
 (2.16) \quad &+ (\Xi(U_\varepsilon^n) \Lambda_\varepsilon(V) \nabla V, \nabla V) + K |\Psi - V|_h^2 + \frac{1}{2} ([\Xi(U_\varepsilon^n)]^2 \Lambda_\varepsilon(V) \nabla W_\varepsilon^n, \nabla V) \\
 &+ \frac{1}{\beta} \left[\frac{1}{\tau_n} (U_\varepsilon^n \lambda_\varepsilon(\Psi), \Psi)^h + \rho_b |(U_\varepsilon^n)^{\frac{1}{2}} \nabla \Psi|_0^2 + \frac{1}{3} ([\Xi(U_\varepsilon^n)]^3 \Lambda_\varepsilon(\Psi) \nabla W_\varepsilon^n, \nabla \Psi) \right. \\
 &\quad \left. + \frac{1}{2} ([\Xi(U_\varepsilon^n)]^{\frac{3}{2}} [\Xi(U_\varepsilon^{n-1})]^{\frac{1}{2}} \Lambda_\varepsilon(\Psi) \nabla V_\varepsilon^{n-1}, \nabla \Psi) \right].
 \end{aligned}$$

From (1.21) and Lemma 2.1 in BGN we have that

$$\begin{aligned}
 (2.17a) \quad &\frac{1}{2} |([\Xi(U_\varepsilon^n)]^2 \Lambda_\varepsilon(V) \nabla W_\varepsilon^n, \nabla V)| \\
 &\leq \frac{1}{2} (\Xi(U_\varepsilon^n) \Lambda_\varepsilon(V) \nabla V, \nabla V) + \frac{1}{8} ([\Xi(U_\varepsilon^n)]^3 \Lambda_\varepsilon(V) \nabla W_\varepsilon^n, \nabla W_\varepsilon^n) \\
 &\leq \frac{1}{2} (\Xi(U_\varepsilon^n) \Lambda_\varepsilon(V) \nabla V, \nabla V) + C(U_\varepsilon^n, W_\varepsilon^n),
 \end{aligned}$$

and similarly, on additionally noting Lemma 2.2 in BN and $U_\varepsilon^n \in S_{>0}^h$, that

$$(2.17b) \quad \frac{1}{3\beta} |([\Xi(U_\varepsilon^n)]^3 \Lambda_\varepsilon(\Psi) \nabla W_\varepsilon^n, \nabla \Psi)| \leq \frac{\rho_b}{4\beta} (U_\varepsilon^n \nabla \Psi, \nabla \Psi) + C(\beta, \rho_b, U_\varepsilon^n, W_\varepsilon^n),$$

$$\begin{aligned}
 (2.17c) \quad &\frac{1}{2} ([\Xi(U_\varepsilon^n)]^{\frac{3}{2}} [\Xi(U_\varepsilon^{n-1})]^{\frac{1}{2}} \Lambda_\varepsilon(\Psi) \nabla V_\varepsilon^{n-1}, \nabla \Psi) \\
 &\leq \frac{\rho_b}{4\beta} (U_\varepsilon^n \nabla \Psi, \nabla \Psi) + C(\beta, \rho_b, U_\varepsilon^{n-1}, U_\varepsilon^n, V_\varepsilon^{n-1}).
 \end{aligned}$$

Moreover, it follows from (1.8) that

$$(2.17d) \quad \frac{1}{\tau_n \beta} |(U_\varepsilon^n \lambda_\varepsilon(\Psi), \Psi)^h| \leq \gamma |\Psi|_h^2 + C(\gamma, \beta, \tau_n, U_\varepsilon^n) \quad \text{for any fixed } \gamma > 0.$$

Combining (2.16) and (2.17)–(2.17d) yields that

$$\begin{aligned}
 \sum_{j \in J} (g_j(\underline{V}, \underline{\Psi}) V_j + g_{j+\mathcal{J}}(\underline{V}, \underline{\Psi}) \Psi_j) &\geq \frac{1}{\tau_n} |V|_h^2 + K |\Psi - V|_h^2 - \gamma |\Psi|_h^2 - C \\
 &\geq \left(\frac{1}{\tau_n} - K_0 \right) |V|_h^2 + \left(\frac{K_0}{2} - \gamma \right) |\Psi|_h^2 - C \\
 (2.18) \quad &\geq \frac{K_0}{4} [|V|_h^2 + |\Psi|_h^2] - C \quad \forall \{V, \Psi\} \in [S^h]^2,
 \end{aligned}$$

where $K_0 \in (0, K]$ and $\gamma \in \mathbb{R}_{>0}$ are chosen sufficiently small. Hence the coerciveness of g follows from (2.18) and (2.1). Therefore, on noting the aforementioned theorem, we have existence of $\{V_\varepsilon^n, \Psi_\varepsilon^n\}$ to (2.5c)–(2.5d) and hence existence of a solution

$\{U_\varepsilon^n, W_\varepsilon^n, V_\varepsilon^n, \Psi_\varepsilon^n\}$ to $(P_\varepsilon^{h,\tau})$. The integral relations follow immediately from choosing $\chi \equiv 1$ in (2.5a), (2.5c), and (2.5d). $\square$

LEMMA 2.4. *Let the assumptions of Theorem 2.3 hold. Then for all $\varepsilon \in (0, 1)$ and for all $h, \tau_n > 0$ a solution $\{U_\varepsilon^n, W_\varepsilon^n, V_\varepsilon^n, \Psi_\varepsilon^n\}$ to the n th step of $(P_\varepsilon^{h,\tau})$ is such that*

$$\begin{aligned}
 & \mathcal{E}(U_\varepsilon^n, V_\varepsilon^n, \Psi_\varepsilon^n) + \frac{c}{2} |U_\varepsilon^n - U_\varepsilon^{n-1}|_1^2 + \frac{1}{2} |V_\varepsilon^n - V_\varepsilon^{n-1}|_h^2 \\
 & + \rho_s \tau_n (\nabla V_\varepsilon^n, \nabla \pi^h[F'_\varepsilon(V_\varepsilon^n)]) + \frac{1}{\beta} \rho_b \tau_n (U_\varepsilon^n \nabla \Psi_\varepsilon^n, \nabla \pi^h[F'_\varepsilon(\Psi_\varepsilon^n)]) \\
 (2.19) \quad & + \tau_n K (\Psi_\varepsilon^n - V_\varepsilon^n, F'_\varepsilon(\Psi_\varepsilon^n) - F'_\varepsilon(V_\varepsilon^n))^h + \frac{\tau_n}{24} ([\Xi(U_\varepsilon^n)]^3 \nabla W_\varepsilon^n, \nabla W_\varepsilon^n) \\
 & + \frac{5}{8} \tau_n (\Xi(U_\varepsilon^n) \nabla V_\varepsilon^n, \nabla V_\varepsilon^n) \\
 & \leq \mathcal{E}(U_\varepsilon^{n-1}, V_\varepsilon^{n-1}, \Psi_\varepsilon^{n-1}) + \frac{\tau_n}{2} (\Xi(U_\varepsilon^{n-1}) \nabla V_\varepsilon^{n-1}, \nabla V_\varepsilon^{n-1}),
 \end{aligned}$$

where $\mathcal{E}(U_\varepsilon^n, V_\varepsilon^n, \Psi_\varepsilon^n) := \frac{c}{2} |U_\varepsilon^n|_1^2 + (\Phi(U_\varepsilon^n) + F_\varepsilon(V_\varepsilon^n), 1)^h + \frac{1}{\beta} (U_\varepsilon^n, \hat{F}_\varepsilon(\Psi_\varepsilon^n))^h$ and $\hat{F}_\varepsilon$ is as defined in (1.15). Furthermore, if $\phi(\cdot)$ satisfies (1.4) with $\nu \geq 7$, then

$$\begin{aligned}
 & (G(U_\varepsilon^n), 1)^h + \frac{\tau_n}{4} (\nabla \pi^h[\phi^+(U_\varepsilon^n)], \nabla U_\varepsilon^n) + \frac{c}{3} \tau_n |\Delta^h U_\varepsilon^n|_h^2 \\
 & \leq (G(U_\varepsilon^{n-1}), 1)^h + \frac{\tau_n}{8} (\nabla \pi^h[\phi^+(U_\varepsilon^{n-1})], \nabla U_\varepsilon^{n-1}) \\
 (2.20) \quad & + C \tau_n [|U_\varepsilon^n|_1^2 + |U_\varepsilon^{n-1}|_1^2] + \frac{\tau_n}{4} (\Xi(U_\varepsilon^{n-1}) \nabla V_\varepsilon^{n-1}, \nabla V_\varepsilon^{n-1}).
 \end{aligned}$$

Proof. First, upon substitution of the trial function $\chi \equiv W_\varepsilon^n$ into the height equation (2.5a), we obtain

$$\begin{aligned}
 & (U_\varepsilon^n - U_\varepsilon^{n-1}, W_\varepsilon^n)^h + \frac{\tau_n}{3} ([\Xi(U_\varepsilon^n)]^3 \nabla W_\varepsilon^n, \nabla W_\varepsilon^n) \\
 (2.21) \quad & = -\frac{\tau_n}{2} ([\Xi(U_\varepsilon^n)]^{\frac{3}{2}} [\Xi(U_\varepsilon^{n-1})]^{\frac{1}{2}} \nabla V_\varepsilon^{n-1}, \nabla W_\varepsilon^n).
 \end{aligned}$$

Substituting $\chi \equiv U_\varepsilon^n - U_\varepsilon^{n-1}$ into (2.5b) and noting the identity $2r(r-s) = (r^2 - s^2) + (r-s)^2$, the convexity of Φ^+ , and the concavity of Φ^- gives

$$\begin{aligned}
 & \frac{c}{2} |U_\varepsilon^n|_1^2 - \frac{c}{2} |U_\varepsilon^{n-1}|_1^2 + \frac{c}{2} |U_\varepsilon^n - U_\varepsilon^{n-1}|_1^2 + (\Phi(U_\varepsilon^n) - \Phi(U_\varepsilon^{n-1}), 1)^h \\
 (2.22) \quad & \leq (W_\varepsilon^n, U_\varepsilon^n - U_\varepsilon^{n-1})^h.
 \end{aligned}$$

Combining (2.21) and (2.22) yields

$$\begin{aligned}
 & \frac{c}{2} |U_\varepsilon^n|_1^2 + (\Phi(U_\varepsilon^n), 1)^h + \frac{\tau_n}{3} ([\Xi(U_\varepsilon^n)]^3 \nabla W_\varepsilon^n, \nabla W_\varepsilon^n) + \frac{c}{2} |U_\varepsilon^n - U_\varepsilon^{n-1}|_1^2 \\
 (2.23) \quad & \leq \frac{c}{2} |U_\varepsilon^{n-1}|_1^2 + (\Phi(U_\varepsilon^{n-1}), 1)^h - \frac{\tau_n}{2} ([\Xi(U_\varepsilon^n)]^{\frac{3}{2}} [\Xi(U_\varepsilon^{n-1})]^{\frac{1}{2}} \nabla V_\varepsilon^{n-1}, \nabla W_\varepsilon^n).
 \end{aligned}$$

Furthermore, choosing $\chi \equiv \pi^h[F'_\varepsilon(V_\varepsilon^n)]$ in the interfacial equation (2.5c) and noting the properties (2.2a)–(2.2b) of Λ_ε yields that

$$\begin{aligned}
 (2.24) \quad & (V_\varepsilon^n - V_\varepsilon^{n-1}, F'_\varepsilon(V_\varepsilon^n))^h + \rho_s \tau_n (\nabla V_\varepsilon^n, \nabla \pi^h[F'_\varepsilon(V_\varepsilon^n)]) \\
 & + \tau_n (\Xi(U_\varepsilon^n) \nabla V_\varepsilon^n, \nabla V_\varepsilon^n) - \tau_n K (\Psi_\varepsilon^n - V_\varepsilon^n, \pi^h[F'_\varepsilon(V_\varepsilon^n)])^h \\
 & = -\frac{\tau_n}{2} ([\Xi(U_\varepsilon^n)]^2 \nabla W_\varepsilon^n, \nabla V_\varepsilon^n).
 \end{aligned}$$

Now $F''_\varepsilon \geq 1$ implies that

$$(2.25) \quad (V_\varepsilon^n - V_\varepsilon^{n-1}, F'_\varepsilon(V_\varepsilon^n))^h \geq (F_\varepsilon(V_\varepsilon^n) - F_\varepsilon(V_\varepsilon^{n-1}), 1)^h + \frac{1}{2} |V_\varepsilon^{n-1} - V_\varepsilon^n|_h^2.$$

Combining (2.24) and (2.25) gives

$$\begin{aligned}
 (2.26) \quad & (F_\varepsilon(V_\varepsilon^n), 1)^h + \frac{1}{2} |V_\varepsilon^{n-1} - V_\varepsilon^n|_h^2 + \rho_s \tau_n (\nabla V_\varepsilon^n, \nabla \pi^h[F'_\varepsilon(V_\varepsilon^n)]) \\
 & + \tau_n (\Xi(U_\varepsilon^n) \nabla V_\varepsilon^n, \nabla V_\varepsilon^n) - \tau_n K (\Psi_\varepsilon^n - V_\varepsilon^n, F'_\varepsilon(V_\varepsilon^n))^h \\
 & \leq (F_\varepsilon(V_\varepsilon^{n-1}), 1)^h - \frac{\tau_n}{2} ([\Xi(U_\varepsilon^n)]^2 \nabla W_\varepsilon^n, \nabla V_\varepsilon^n).
 \end{aligned}$$

Similarly, choosing $\chi \equiv \pi^h[F'_\varepsilon(\Psi_\varepsilon^n)]$ in the bulk chemical equation (2.5d) and using the properties (2.2a)–(2.2b) gives

$$\begin{aligned}
 & (U_\varepsilon^n \lambda_\varepsilon(\Psi_\varepsilon^n) - U_\varepsilon^{n-1} \lambda_\varepsilon(\Psi_\varepsilon^{n-1}), F'_\varepsilon(\Psi_\varepsilon^n))^h + \tau_n \rho_b (U_\varepsilon^n \nabla \Psi_\varepsilon^n, \nabla \pi^h[F'_\varepsilon(\Psi_\varepsilon^n)]) \\
 & + \frac{\tau_n}{3} ([\Xi(U_\varepsilon^n)]^3 \nabla W_\varepsilon^n, \nabla \Psi_\varepsilon^n) + \tau_n \beta K (\Psi_\varepsilon^n - V_\varepsilon^n, F'_\varepsilon(\Psi_\varepsilon^n))^h \\
 & = -\frac{\tau_n}{2} ([\Xi(U_\varepsilon^n)]^{\frac{3}{2}} [\Xi(U_\varepsilon^{n-1})]^{\frac{1}{2}} \nabla V_\varepsilon^{n-1}, \nabla \Psi_\varepsilon^n).
 \end{aligned}$$

Combining this with the height equation (2.5a) for $\chi \equiv \Psi_\varepsilon^n$ gives

$$\begin{aligned}
 (2.27) \quad & (U_\varepsilon^n \lambda_\varepsilon(\Psi_\varepsilon^n) - U_\varepsilon^{n-1} \lambda_\varepsilon(\Psi_\varepsilon^{n-1}), F'_\varepsilon(\Psi_\varepsilon^n))^h - (U_\varepsilon^n - U_\varepsilon^{n-1}, \Psi_\varepsilon^n)^h \\
 & = -\tau_n \rho_b (U_\varepsilon^n \nabla \Psi_\varepsilon^n, \nabla \pi^h[F'_\varepsilon(\Psi_\varepsilon^n)]) - \tau_n \beta K (\Psi_\varepsilon^n - V_\varepsilon^n, F'_\varepsilon(\Psi_\varepsilon^n))^h.
 \end{aligned}$$

We recall (1.15) and (1.16) and also note that $(U_\varepsilon^n - U_\varepsilon^{n-1}, 1)^h = 0$, which follows from inserting $\chi \equiv 1$ into (2.5a). Then the left-hand side of (2.27) may be rewritten as

$$\begin{aligned}
 & (U_\varepsilon^n \lambda_\varepsilon(\Psi_\varepsilon^n) - U_\varepsilon^{n-1} \lambda_\varepsilon(\Psi_\varepsilon^{n-1}), F'_\varepsilon(\Psi_\varepsilon^n))^h - (U_\varepsilon^n - U_\varepsilon^{n-1}, \Psi_\varepsilon^n)^h \\
 & = (U_\varepsilon^n - U_\varepsilon^{n-1}, \lambda_\varepsilon(\Psi_\varepsilon^n) F'_\varepsilon(\Psi_\varepsilon^n) - \Psi_\varepsilon^n)^h + (\lambda_\varepsilon(\Psi_\varepsilon^n) - \lambda_\varepsilon(\Psi_\varepsilon^{n-1}), U_\varepsilon^{n-1} F'_\varepsilon(\Psi_\varepsilon^n))^h \\
 & \geq (U_\varepsilon^n - U_\varepsilon^{n-1}, \widehat{F}_\varepsilon(\Psi_\varepsilon^n) - 1)^h + (\widehat{F}_\varepsilon(\Psi_\varepsilon^n) - \widehat{F}_\varepsilon(\Psi_\varepsilon^{n-1}), U_\varepsilon^{n-1})^h \\
 & = (U_\varepsilon^n \widehat{F}_\varepsilon(\Psi_\varepsilon^n) - U_\varepsilon^{n-1} \widehat{F}_\varepsilon(\Psi_\varepsilon^{n-1}), 1)^h,
 \end{aligned}$$

and thus

$$\begin{aligned}
 (2.28) \quad & (U_\varepsilon^n \widehat{F}_\varepsilon(\Psi_\varepsilon^n) - U_\varepsilon^{n-1} \widehat{F}_\varepsilon(\Psi_\varepsilon^{n-1}), 1)^h \\
 & \leq -\tau_n \rho_b (U_\varepsilon^n \nabla \Psi_\varepsilon^n, \nabla \pi^h[F'_\varepsilon(\Psi_\varepsilon^n)]) - \tau_n \beta K (\Psi_\varepsilon^n - V_\varepsilon^n, F'_\varepsilon(\Psi_\varepsilon^n))^h.
 \end{aligned}$$

Combining (2.23), (2.26), and (2.28) and noting Young's inequality (1.21) yields that

$$\begin{aligned}
& \mathcal{E}(U_\varepsilon^n, V_\varepsilon^n, \Psi_\varepsilon^n) + \frac{c}{2} \|U_\varepsilon^n - U_\varepsilon^{n-1}\|_1^2 + \frac{1}{2} \|V_\varepsilon^n - V_\varepsilon^{n-1}\|_h^2 + \rho_s \tau_n (\nabla V_\varepsilon^n, \nabla \pi^h[F'_\varepsilon(V_\varepsilon^n)]) \\
& + \frac{1}{\beta} \tau_n \rho_b (U_\varepsilon^n \nabla \Psi_\varepsilon^n, \nabla \pi^h[F'_\varepsilon(\Psi_\varepsilon^n)]) + \tau_n K (\Psi_\varepsilon^n - V_\varepsilon^n, F'_\varepsilon(\Psi_\varepsilon^n) - F'_\varepsilon(V_\varepsilon^n))^h \\
& + \frac{\tau_n}{3} ([\Xi(U_\varepsilon^n)]^3 \nabla W_\varepsilon^n, \nabla W_\varepsilon^n) + \tau_n (\Xi(U_\varepsilon^n) \nabla V_\varepsilon^n, \nabla V_\varepsilon^n) \\
& \leq \mathcal{E}(U_\varepsilon^{n-1}, V_\varepsilon^{n-1}, \Psi_\varepsilon^{n-1}) - \frac{\tau_n}{2} ([\Xi(U_\varepsilon^n)]^2 \nabla W_\varepsilon^n, \nabla V_\varepsilon^n) \\
& - \frac{\tau_n}{2} ([\Xi(U_\varepsilon^n)]^{\frac{3}{2}} [\Xi(U_\varepsilon^{n-1})]^{\frac{1}{2}} \nabla W_\varepsilon^n, \nabla V_\varepsilon^{n-1}) \\
& \leq \mathcal{E}(U_\varepsilon^{n-1}, V_\varepsilon^{n-1}, \Psi_\varepsilon^{n-1}) + \frac{\zeta + \gamma}{4} \tau_n ([\Xi(U_\varepsilon^n)]^3 \nabla W_\varepsilon^n, \nabla W_\varepsilon^n) \\
& + \frac{\tau_n}{4\zeta} (\Xi(U_\varepsilon^{n-1}) \nabla V_\varepsilon^{n-1}, \nabla V_\varepsilon^{n-1}) + \frac{\tau_n}{4\gamma} (\Xi(U_\varepsilon^n) \nabla V_\varepsilon^n, \nabla V_\varepsilon^n)
\end{aligned}$$

for arbitrary choices of $\zeta, \gamma > 0$. Choosing $\zeta = \frac{1}{2}$ and $\gamma = \frac{2}{3}$ leads to the desired result for the discrete energy structure (2.19).

The desired result (2.20) was derived in Lemma 2.4 in BN. $\square$

Remark 2.5. We note that (2.19) and (2.20) are the discrete analogues of the formal energy estimates (1.20) (on noting (1.22)) and (1.24), respectively.

THEOREM 2.6. *Let $\phi(\cdot)$ satisfy (1.4) with $\delta > 0$. Let the assumptions (A) hold and $\{U_\varepsilon^0, V_\varepsilon^0, \Psi_\varepsilon^0\} \in S_{>0}^h \times [S^h]^2$. Then for all $\varepsilon \in (0, 1)$, $h > 0$ and for all time partitions $\{\tau_n\}_{n=1}^N$ a solution $\{U_\varepsilon^n, W_\varepsilon^n, V_\varepsilon^n, \Psi_\varepsilon^n\}_{n=1}^N$ to $(P_\varepsilon^{h,\tau})$ is such that $\mathcal{f}U_\varepsilon^n = \mathcal{f}U_\varepsilon^0$ and $\mathcal{f}(V_\varepsilon^n + \frac{1}{\beta} \pi^h[U_\varepsilon^n \lambda_\varepsilon(\Psi_\varepsilon^n)]) = \mathcal{f}(V_\varepsilon^0 + \frac{1}{\beta} \pi^h[U_\varepsilon^0 \lambda_\varepsilon(\Psi_\varepsilon^0)])$, $n = 1 \rightarrow N$, and if $\tau_n \leq \frac{5}{4} \omega \tau_{n-1}$, $n = 2 \rightarrow N$, for an $\omega \in (0, 1)$, then*

$$\begin{aligned}
& c \max_{n=1 \rightarrow N} \|U_\varepsilon^n\|_1^2 + \max_{n=1 \rightarrow N} (\Phi(U_\varepsilon^n), 1)^h + \max_{n=1 \rightarrow N} (F_\varepsilon(V_\varepsilon^n), 1)^h \\
& + c \sum_{n=1}^N \|U_\varepsilon^n - U_\varepsilon^{n-1}\|_1^2 + \sum_{n=1}^N \|V_\varepsilon^n - V_\varepsilon^{n-1}\|_0^2 \\
(2.29a) \quad & + \rho_s \sum_{n=1}^N \tau_n (\nabla V_\varepsilon^n, \nabla \pi^h[F'_\varepsilon(V_\varepsilon^n)]) + \sum_{n=1}^N \tau_n ([\Xi(U_\varepsilon^n)]^3 \nabla W_\varepsilon^n, \nabla W_\varepsilon^n) \\
& + (1 - \omega) \sum_{n=1}^N \tau_n (\Xi(U_\varepsilon^n) \nabla V_\varepsilon^n, \nabla V_\varepsilon^n) + \rho_b \sum_{n=1}^N \tau_n (U_\varepsilon^n \nabla \Psi_\varepsilon^n, \nabla \Psi_\varepsilon^n) \\
& + K \sum_{n=1}^N \tau_n (\Psi_\varepsilon^n - V_\varepsilon^n, F'_\varepsilon(\Psi_\varepsilon^n) - F'_\varepsilon(V_\varepsilon^n))^h \leq C \mathcal{C}^0,
\end{aligned}$$

where

$$(2.29b) \quad \mathcal{C}^0 := 1 + \|U_\varepsilon^0\|_1^2 + (\Phi(U_\varepsilon^0) + F_\varepsilon(V_\varepsilon^0), 1)^h + (U_\varepsilon^0, \widehat{F}_\varepsilon(\Psi_\varepsilon^0))^h + (\Xi(U_\varepsilon^0) \nabla V_\varepsilon^0, \nabla V_\varepsilon^0).$$

In addition,

$$(2.30) \quad \begin{aligned} & \max_{n=1 \rightarrow N} |V_\varepsilon^n|_0^2 + \varepsilon^{-1} \max_{n=1 \rightarrow N} |\pi^h[V_\varepsilon^n]_-|_0^2 + \rho_s \sum_{n=1}^N \tau_n \|V_\varepsilon^n\|_1^2 + K \sum_{n=1}^N \tau_n |\Psi_\varepsilon^n - V_\varepsilon^n|_0^2 \\ & + \sum_{n=1}^N \tau_n [(F_\varepsilon(\Psi_\varepsilon^n), 1)^h + |\Psi_\varepsilon^n|_0^2 + \varepsilon^{-1} |\pi^h[\Psi_\varepsilon^n]_-|_0^2] \leq C \mathcal{C}^0, \end{aligned}$$

and, on letting $B_\varepsilon^n := \pi^h[U_\varepsilon^n \lambda_\varepsilon(\Psi_\varepsilon^n)]$, $n = 0 \rightarrow N$, we have that

$$(2.31a) \quad \begin{aligned} & \sum_{n=1}^N \tau_n \left[\left\| \mathcal{G} \left[\frac{U_\varepsilon^n - U_\varepsilon^{n-1}}{\tau_n} \right] \right\|_{1,q}^2 + \left\| \mathcal{G} \left[\frac{V_\varepsilon^n - V_\varepsilon^{n-1}}{\tau_n} \right] \right\|_{1,q}^2 + \left\| \mathcal{G} \left[\frac{B_\varepsilon^n - B_\varepsilon^{n-1}}{\tau_n} \right] \right\|_{1,q}^2 \right] \\ & + \sum_{n=1}^N \tau_n \|B_\varepsilon^n\|_{1,q}^2 \leq C \left(\max_{n=0 \rightarrow N} \{ |\Xi(U_\varepsilon^n)|^3|_{0,r}, |(U_\varepsilon^n)^{\frac{1}{2}}|_{0,r} \} \right) \mathcal{C}^0, \end{aligned}$$

where $q = 2$ and $r = \infty$ if $d = 1$, $q \in (1, 2)$; and $r = \frac{2q}{2-q}$ if $d = 2$; and

$$(2.31b) \quad |\Xi(U_\varepsilon^n)|^{\alpha}|_{0,s} \leq C \|U_\varepsilon^n\|_1^{\alpha} \quad \forall \alpha \in (0, \infty), \quad \forall s \in \begin{cases} [1, \infty] & \text{if } d = 1, \\ [1, \infty) & \text{if } d = 2. \end{cases}$$

Furthermore, if $\phi(\cdot)$ satisfies (1.4) with $\nu \geq 7$, then

$$(2.32) \quad \begin{aligned} & \max_{n=1 \rightarrow N} (G(U_\varepsilon^n), 1)^h + c \sum_{n=1}^N \tau_n |\Delta^h U_\varepsilon^n|_h^2 + \sum_{n=1}^N \tau_n (\nabla \pi^h[\phi^+(U_\varepsilon^n)], \nabla U_\varepsilon^n) \\ & \leq C [\mathcal{C}^0 + (G(U_\varepsilon^0), 1)^h + (\nabla \pi^h[\phi^+(U_\varepsilon^0)], \nabla U_\varepsilon^0)]. \end{aligned}$$

Proof. Summing the discrete energy estimate (2.19) from $n = 1 \rightarrow k$ and using $\tau_n \leq \frac{5}{4} \omega \tau_{n-1}$, $n = 2 \rightarrow k$, yields for any $k \leq N$ that

$$(2.33) \quad \begin{aligned} & \mathcal{E}(U_\varepsilon^k, V_\varepsilon^k, \Psi_\varepsilon^k) + \frac{1}{2} \sum_{n=1}^k [c |U_\varepsilon^n - U_\varepsilon^{n-1}|_1^2 + |V_\varepsilon^n - V_\varepsilon^{n-1}|_h^2] \\ & + \rho_s \sum_{n=1}^k \tau_n (\nabla V_\varepsilon^n, \nabla \pi^h[F'_\varepsilon(V_\varepsilon^n)]) + \frac{1}{\beta} \rho_b \sum_{n=1}^k \tau_n (U_\varepsilon^n \nabla \Psi_\varepsilon^n, \nabla \pi^h[F'_\varepsilon(\Psi_\varepsilon^n)]) \\ & + \sum_{n=1}^k \tau_n \left[K (\Psi_\varepsilon^n - V_\varepsilon^n, F'_\varepsilon(\Psi_\varepsilon^n) - F'_\varepsilon(V_\varepsilon^n))^h + \frac{1}{24} ([\Xi(U_\varepsilon^n)]^3 \nabla W_\varepsilon^n, \nabla W_\varepsilon^n) \right] \\ & + \frac{5}{8} (1 - \omega) \sum_{n=1}^k \tau_n (\Xi(U_\varepsilon^n) \nabla V_\varepsilon^n, \nabla V_\varepsilon^n) \\ & \leq \mathcal{E}(U_\varepsilon^0, V_\varepsilon^0, \Psi_\varepsilon^0) + \frac{\tau_1}{2} (\Xi(U_\varepsilon^0) \nabla V_\varepsilon^0, \nabla V_\varepsilon^0). \end{aligned}$$

Similarly to (2.14), it holds that

$$(2.34) \quad (U_\varepsilon^n \nabla z^h, \nabla \pi^h[F'_\varepsilon(z^h)]) \geq |(U_\varepsilon^n)^{\frac{1}{2}} \nabla z^h|_0^2 \quad \forall z^h \in S^h.$$

Therefore, on noting (1.13), (2.4), (2.1), (2.10), (2.34), and a Poincaré inequality, the bounds (2.29a) follow directly from (2.33).

Combining the third bound in (2.29a) and (1.13) yields the first two bounds in (2.30). These, together with the sixth bound in (2.29a), yield, on noting (2.14), the third bound in (2.30). Moreover, the fourth bound in (2.30) follows from (1.11) and the last bound in (2.29a). We will now prove the final three bounds in (2.30). First, by the convexity of F_ε , we have for all $r, s \in \mathbb{R}$ that

(2.35)

$$F_\varepsilon(r) \leq F_\varepsilon(s) + (r-s) F'_\varepsilon(r) = F_\varepsilon(s) + (r-s) (F'_\varepsilon(r) - F'_\varepsilon(s)) + (r-s) F'_\varepsilon(s).$$

The last term on the right-hand side of (2.35) is only nonnegative if either $r \leq s \leq 1$ or $r \geq s \geq 1$, in which case we have that

(2.36)

$$2(r-s) F'_\varepsilon(s) \leq F''_\varepsilon(s) (r-s)^2 + \frac{[F'_\varepsilon(s)]^2}{F''_\varepsilon(s)} \leq (r-s) (F'_\varepsilon(r) - F'_\varepsilon(s)) + \frac{[F'_\varepsilon(s)]^2}{F''_\varepsilon(s)}.$$

The fifth bound in (2.30) then follows from (2.35), (2.36), (2.29a), (1.14), and the first two bounds in (2.30). This, together with (1.13), then yields the last two bounds in (2.30).

From (1.25), (2.5c), Lemma 2.1 in BGN, and (2.13) we obtain that

$$\begin{aligned} & \left(\nabla \mathcal{G} \left[\frac{V_\varepsilon^n - V_\varepsilon^{n-1}}{\tau_n} \right], \nabla \eta \right) + \left(\mathcal{G} \left[\frac{V_\varepsilon^n - V_\varepsilon^{n-1}}{\tau_n} \right], \eta \right) = \left(\frac{V_\varepsilon^n - V_\varepsilon^{n-1}}{\tau_n}, Q^h \eta \right)^h \\ & = -\rho_s (\nabla V_\varepsilon^n, \nabla Q^h \eta) - \left(\Xi(U_\varepsilon^n) \Lambda_\varepsilon(V_\varepsilon^n) \nabla V_\varepsilon^n \right. \\ (2.37) \quad & \left. + \frac{1}{2} [\Xi(U_\varepsilon^n)]^2 \Lambda_\varepsilon(V_\varepsilon^n) \nabla W_\varepsilon^n, \nabla Q^h \eta \right) + K (\Psi_\varepsilon^n - V_\varepsilon^n, Q^h \eta)^h \\ & \leq C [\rho_s |\nabla V_\varepsilon^n|_0 + |\Xi(U_\varepsilon^n)]^{\frac{1}{2}}|_{0,r} (|\Xi(U_\varepsilon^n)]^{\frac{1}{2}} \nabla V_\varepsilon^n|_0 \\ & \quad + |\Xi(U_\varepsilon^n)]^{\frac{3}{2}} \nabla W_\varepsilon^n|_0) |\eta|_{1,q'} + C K |\Psi_\varepsilon^n - V_\varepsilon^n|_0 |\eta|_{0,q'}. \end{aligned}$$

In a similar fashion, it follows from (2.5d) that

(2.38)

$$\begin{aligned} & \left(\nabla \mathcal{G} \left[\frac{B_\varepsilon^n - B_\varepsilon^{n-1}}{\tau_n} \right], \nabla \eta \right) + \left(\mathcal{G} \left[\frac{B_\varepsilon^n - B_\varepsilon^{n-1}}{\tau_n} \right], \eta \right) \\ & = \left(\frac{U_\varepsilon^n \lambda_\varepsilon(\Psi_\varepsilon^n) - U_\varepsilon^{n-1} \lambda_\varepsilon(\Psi_\varepsilon^{n-1})}{\tau_n}, Q^h \eta \right)^h \\ & = -\rho_b (U_\varepsilon^n \nabla \Psi_\varepsilon^n, \nabla Q^h \eta) - \frac{1}{3} ([\Xi(U_\varepsilon^n)]^3 \Lambda_\varepsilon(\Psi_\varepsilon^n) \nabla W_\varepsilon^n, \nabla Q^h \eta) \\ & \quad - \beta K (\Psi_\varepsilon^n - V_\varepsilon^n, Q^h \eta)^h - \frac{1}{2} ([\Xi(U_\varepsilon^n)]^{\frac{3}{2}} [\Xi(U_\varepsilon^{n-1})]^{\frac{1}{2}} \Lambda_\varepsilon(\Psi_\varepsilon^n) \nabla V_\varepsilon^{n-1}, \nabla Q^h \eta) \\ & \leq C [|\Xi(U_\varepsilon^n)]^{\frac{3}{2}}|_{0,r} (|\Xi(U_\varepsilon^{n-1})|^{\frac{1}{2}} \nabla V_\varepsilon^{n-1}|_0 + |\Xi(U_\varepsilon^n)]^{\frac{3}{2}} \nabla W_\varepsilon^n|_0) \\ & \quad + \rho_b |(U_\varepsilon^n)^{\frac{1}{2}}|_{0,r} |(U_\varepsilon^n)^{\frac{1}{2}} \nabla \Psi_\varepsilon^n|_0 |\eta|_{1,q'} + C \beta K |\Psi_\varepsilon^n - V_\varepsilon^n|_0 |\eta|_{0,q'}. \end{aligned}$$

Moreover, it follows from (2.9) and (1.8) that

$$\begin{aligned}
 \|B_\varepsilon^n\|_{1,q} &\leq C \left[|U_\varepsilon^n \pi^h[\lambda_\varepsilon(\Psi_\varepsilon^n)]|_{0,q} + |U_\varepsilon^n \nabla \pi^h[\lambda_\varepsilon(\Psi_\varepsilon^n)]|_{0,q} + |\pi^h[\lambda_\varepsilon(\Psi_\varepsilon^n)] \nabla U_\varepsilon^n|_{0,q} \right] \\
 &\leq C \left[\|U_\varepsilon^n\|_1 + |(U_\varepsilon^n)^{\frac{1}{2}}|_{0,r} |(U_\varepsilon^n)^{\frac{1}{2}} \nabla \Psi_\varepsilon^n|_0 \right].
 \end{aligned}
 \tag{2.39}$$

Combining (2.37), a similar bound for the discrete U_ε time derivative (see [6, (2.73)]), (2.38), (2.39), the assumptions on τ_n , and the bounds (2.29a) and (2.30) yields the bounds (2.31a).

The desired result (2.31b) was proved in Theorem 2.2 in BN.

Finally, summing (2.20) from $n = 1 \rightarrow k$, observing that $\tau_n \leq \frac{5}{4} \omega \tau_{n-1}$, $n = 2 \rightarrow k$, and noting the first and eighth bounds in (2.29a) yields (2.32). $\square$

Remark 2.7. We note that all the results in this section hold also in the absence of attractive van der Waals forces, $a = 0$. The same holds true for the results quoted from BN, even though it was not explicitly stated there.

LEMMA 2.8. *Let $u^0, v^0, \psi^0 \in H_{\geq 0}^1(\Omega)$, with $u^0 \in L^\infty(\Omega)$ and $u^0(x) \geq \zeta > 0$ for a.e. $x \in \Omega$, and let the assumptions (A) hold. On choosing either $\{U_\varepsilon^0, V_\varepsilon^0, \Psi_\varepsilon^0\} \equiv \{Q^h u^0, Q^h v^0, Q^h \psi^0\}$ or $\{U_\varepsilon^0, V_\varepsilon^0, \Psi_\varepsilon^0\} \equiv \{\pi^h u^0, \pi^h v^0, \pi^h \psi^0\}$ if either $d = 1$ or $\{u^0, v^0, \psi^0\} \in [W^{1,e}(\Omega)]^3$ with $e > 2$, it follows that $\{U_\varepsilon^0, V_\varepsilon^0, \Psi_\varepsilon^0\} \in [S_{\geq 0}^h]^3$ with $U_\varepsilon^0 \geq \zeta$ are such that for all $h > 0$*

$$\mathcal{C}^0 + (G(U_\varepsilon^0), 1)^h + (\nabla \pi^h[\phi^+(U_\varepsilon^0)], \nabla U_\varepsilon^0) \leq C.
 \tag{2.40}$$

Proof. The desired result (2.40) follows immediately from (2.29b), (2.12), (2.8), (2.13), (2.3), (1.12), (1.23), (1.4), and Lemma 2.2 in BN. $\square$

3. Convergence. Let

$$U_\varepsilon(t) := \frac{t - t_{n-1}}{\tau_n} U_\varepsilon^n + \frac{t_n - t}{\tau_n} U_\varepsilon^{n-1}, \quad t \in [t_{n-1}, t_n], \quad n \geq 1,
 \tag{3.1a}$$

and

$$U_\varepsilon^+(t) := U_\varepsilon^n, \quad U_\varepsilon^-(t) := U_\varepsilon^{n-1}, \quad t \in (t_{n-1}, t_n], \quad n \geq 1.
 \tag{3.1b}$$

We note for future reference that

$$U_\varepsilon - U_\varepsilon^\pm = (t - t_n^\pm) \frac{\partial U_\varepsilon}{\partial t}, \quad t \in (t_{n-1}, t_n), \quad n \geq 1,
 \tag{3.2}$$

where $t_n^+ := t_n$ and $t_n^- := t_{n-1}$. We introduce also $\bar{\tau}(t) := \tau_n$ for $t \in (t_{n-1}, t_n]$, $n \geq 1$.

Using the above notation, and introducing analogous notation for $W_\varepsilon, V_\varepsilon, \Psi_\varepsilon$, and B_ε (recall (2.31a)), $(P_\varepsilon^{h,\tau})$ can be restated as follows.

Find $\{U_\varepsilon, W_\varepsilon^+, V_\varepsilon, \Psi_\varepsilon\} \in C([0, T]; S^h) \times L^\infty(0, T; S^h) \times [C([0, T]; S^h)]^2$ such that

for all $\chi \in L^2(0, T; S^h)$

$$\begin{aligned}
 & \int_0^T \left[\left(\frac{\partial U_\varepsilon}{\partial t}, \chi \right)^h + \frac{1}{3} ([\Xi(U_\varepsilon^+)]^3 \nabla W_\varepsilon^+, \nabla \chi) \right] dt \\
 (3.3a) \quad & = -\frac{1}{2} \int_0^T ([\Xi(U_\varepsilon^+)]^{\frac{3}{2}} [\Xi(U_\varepsilon^-)]^{\frac{1}{2}} \nabla V_\varepsilon^-, \nabla \chi) dt, \\
 & \int_0^T \left[\left(\frac{\partial V_\varepsilon}{\partial t}, \chi \right)^h + \rho_s (\nabla V_\varepsilon^+, \nabla \chi) + (\Xi(U_\varepsilon^+) \Lambda_\varepsilon(V_\varepsilon^+) \nabla V_\varepsilon^+, \nabla \chi) \right. \\
 (3.3b) \quad & \left. - K(\Psi_\varepsilon^+ - V_\varepsilon^+, \chi)^h \right] dt = -\frac{1}{2} \int_0^T ([\Xi(U_\varepsilon^+)]^2 \Lambda_\varepsilon(V_\varepsilon^+) \nabla W_\varepsilon^+, \nabla \chi) dt, \\
 & \int_0^T \left[\left(\frac{\partial B_\varepsilon}{\partial t}, \chi \right)^h + \rho_b (U_\varepsilon^+ \nabla \Psi_\varepsilon^+, \nabla \chi) + \frac{1}{3} ([\Xi(U_\varepsilon^+)]^3 \Lambda_\varepsilon(\Psi_\varepsilon^+) \nabla W_\varepsilon^+, \nabla \chi) \right. \\
 & \left. + \beta K(\Psi_\varepsilon^+ - V_\varepsilon^+, \chi)^h \right] dt \\
 (3.3c) \quad & = -\frac{1}{2} \int_0^T ([\Xi(U_\varepsilon^+)]^{\frac{3}{2}} [\Xi(U_\varepsilon^-)]^{\frac{1}{2}} \Lambda_\varepsilon(\Psi_\varepsilon^+) \nabla V_\varepsilon^-, \nabla \chi) dt,
 \end{aligned}$$

where for a.a. $t \in (0, T)$ and for all $z^h \in S^h$

$$(3.3d) \quad (W_\varepsilon^+(\cdot, t), z^h)^h = c(\nabla U_\varepsilon^+(\cdot, t), \nabla z^h) + (\phi^+(U_\varepsilon^+(\cdot, t)) + \phi^-(U_\varepsilon^-(\cdot, t)), z^h)^h;$$

that is, $W_\varepsilon^+ \equiv -c \Delta^h U_\varepsilon^+ + \pi^h[\phi^+(U_\varepsilon^+) + \phi^-(U_\varepsilon^-)]$.

LEMMA 3.1. Let $\rho_s > 0$, $\phi(\cdot)$ satisfy (1.4) with $\delta > 0$, and $u^0 \in H^1(\Omega) \cap L^\infty(\Omega)$ with $u^0 \geq \zeta > 0$ a.e. and $v^0, \psi^0 \in H_{\geq 0}^1(\Omega)$. Let $\{\mathcal{T}^h, U_\varepsilon^0, V_\varepsilon^0, \Psi_\varepsilon^0, \{\tau_n\}_{n=1}^N, \varepsilon\}_{h>0}$ be such that

- (i) either $\{U_\varepsilon^0, V_\varepsilon^0, \Psi_\varepsilon^0\} \equiv \{Q^h u^0, Q^h v^0, Q^h \psi^0\}$ or $\{U_\varepsilon^0, V_\varepsilon^0, \Psi_\varepsilon^0\} \equiv \{\pi^h u^0, \pi^h v^0, \pi^h \psi^0\}$ if either $d = 1$ or $\{u^0, v^0, \psi^0\} \in [W^{1,e}(\Omega)]^3$ with $e > 2$;
- (ii) Ω and $\{\mathcal{T}^h\}_{h>0}$ fulfill assumption (A), $\varepsilon \in (0, 1)$, and $\tau_n \leq \frac{5}{4} \omega \tau_{n-1}$, $n = 2 \rightarrow N$, for an $\omega \in (0, 1)$;
- (iii) $\tau h^{-d(1-\frac{2}{p})} \rightarrow 0$ and $\varepsilon h^{-d(\frac{1}{2}-\frac{1}{p})} \rightarrow 0$ as $h \rightarrow 0$, where $p = 2$ if $d = 1$ and $p > 2$ if $d = 2$.

Then there exist a subsequence of $\{U_\varepsilon, W_\varepsilon^+, V_\varepsilon, \Psi_\varepsilon\}_h$, where $\{U_\varepsilon, W_\varepsilon^+, V_\varepsilon, \Psi_\varepsilon\}$ solve $(P_\varepsilon^{h,\tau})$, and functions

$$(3.4a) \quad u \in L^\infty(0, T; H_{\geq 0}^1(\Omega)) \cap H^1(0, T; (W^{1,q'}(\Omega))'),$$

$$(3.4b) \quad v \in L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; H_{\geq 0}^1(\Omega)) \cap H^1(0, T; (W^{1,q'}(\Omega))'),$$

$$(3.4c) \quad \psi \in L^2(0, T; L_{\geq 0}^2(\Omega)), \text{ such that}$$

$$(3.4d) \quad \lambda(v), \lambda(\psi) \in L^\infty(\Omega_T),$$

with $u(\cdot, 0) = u^0(\cdot)$ in Y_1 , $v(\cdot, 0) = v^0(\cdot)$ in Y_2 , where $H^1(\Omega) \xhookrightarrow{c} Y_1$, $L^2(\Omega) \xhookrightarrow{c} Y_2$, and $\int u(\cdot, t) = \int u^0 > 0$, $\int [v(\cdot, t) + \frac{1}{\beta} u(\cdot, t) \lambda(\psi(\cdot, t))] = \int [v^0 + \frac{1}{\beta} u^0 \lambda(\psi^0)]$ for a.a. $t \in (0, T)$ such that as $h \rightarrow 0$

$$\begin{aligned}
(3.5a) \quad & U_\varepsilon, U_\varepsilon^\pm \rightarrow u && \text{weak-* in } L^\infty(0, T; H^1(\Omega)), \\
(3.5b) \quad & V_\varepsilon, V_\varepsilon^\pm \rightarrow v && \text{weak-* in } L^\infty(0, T; L^2(\Omega)), \text{ weakly in } L^2(0, T; H^1(\Omega)), \\
(3.5c) \quad & \Psi_\varepsilon^+ \rightarrow \psi && \text{weakly in } L^2(\Omega_T), \\
(3.5d) \quad & \mathcal{G} \frac{\partial U_\varepsilon}{\partial t} \rightarrow \mathcal{G} \frac{\partial u}{\partial t} \quad \text{and} \quad \mathcal{G} \frac{\partial V_\varepsilon}{\partial t} \rightarrow \mathcal{G} \frac{\partial v}{\partial t} && \text{weakly in } L^2(0, T; W^{1,q}(\Omega)), \\
(3.6a) \quad & (U_\varepsilon)^\alpha, (U_\varepsilon^\pm)^\alpha \rightarrow u^\alpha \quad \text{for any } \alpha \in (0, \infty), && \text{strongly in } L^2(0, T; L^s(\Omega)), \\
(3.6b) \quad & V_\varepsilon, V_\varepsilon^\pm \rightarrow v && \text{strongly in } L^2(0, T; L^p(\Omega)), \\
(3.7a) \quad & [\Xi(U_\varepsilon^\pm)]^\alpha \rightarrow u^\alpha \mathcal{I} \quad \text{for any } \alpha \in (0, \infty), && \text{strongly in } L^2(0, T; L^s(\Omega)), \\
(3.7b) \quad & \Lambda_\varepsilon(V_\varepsilon^+) \rightarrow \lambda(v) \mathcal{I} && \text{strongly in } L^2(0, T; L^p(\Omega)),
\end{aligned}$$

where $s \in [2, \infty]$ and $q = 2$ if $d = 1$, $s \in [2, \infty)$, and $q \in (1, 2)$ if $d = 2$.

Furthermore, if $d = 1$, or $d = 2$ and $\nu \geq 7$ in (1.4), then u in addition to (3.4a) satisfies

$$(3.8) \quad u \in L^2(0, T; H^2(\Omega)),$$

and there exists a subsequence of $\{U_\varepsilon, W_\varepsilon^+, V_\varepsilon, \Psi_\varepsilon\}_h$ satisfying (3.5a)–(3.5d), (3.6a)–(3.6b), (3.7a)–(3.7b), and as $h \rightarrow 0$

$$\begin{aligned}
(3.9a) \quad & \Delta^h U_\varepsilon^+ \rightarrow \Delta u && \text{weakly in } L^2(\Omega_T), \\
(3.9b) \quad & U_\varepsilon, U_\varepsilon^\pm \rightarrow u && \text{weakly in } L^2(0, T; W^{1,p}(\Omega)), \\
(3.9c) \quad & U_\varepsilon, U_\varepsilon^\pm \rightarrow u && \text{strongly in } L^2(0, T; C^{0,\gamma}(\bar{\Omega})) \quad \text{for any } \gamma \in (0, 1 - \frac{d}{p}),
\end{aligned}$$

and for a.a. $t \in (0, T)$

$$(3.9d) \quad u(\cdot, t) \in C^{0,\gamma}(\bar{\Omega}) \quad \text{with} \quad u(x, t) \geq \zeta(t) > 0 \quad \forall x \in \bar{\Omega}.$$

On extracting a further subsequence, it also holds as $h \rightarrow 0$ that for a.a. $t \in (0, T)$

$$\begin{aligned}
(3.10a) \quad & \pi^h[\phi^\pm(U_\varepsilon^\pm)](\cdot, t) \rightarrow \phi^\pm(u(\cdot, t)) && \text{strongly in } C(\bar{\Omega}), \\
(3.10b) \quad & W_\varepsilon^+(\cdot, t) \rightarrow w(\cdot, t) \equiv -c \Delta u(\cdot, t) + \phi(u(\cdot, t)) && \text{weakly in } H^1(\Omega), \\
(3.10c) \quad & [\Xi(U_\varepsilon^+)]^{\frac{3}{2}} \nabla W_\varepsilon^+ \rightarrow u^{\frac{3}{2}} \nabla w && \text{weakly in } L^2(\Omega_T).
\end{aligned}$$

Moreover, we have that

$$(3.11) \quad U_\varepsilon, U_\varepsilon^\pm \rightarrow u \quad \text{strongly in } L^2(0, T; H^1(\Omega)).$$

Proof. Noting the definitions (3.1a)–(3.1b) and [6, (1.19)], the bounds in (2.29a)–

(2.31b) together with (2.40) and our assumption (i) imply that

(3.12)

$$\begin{aligned}
& \|U_\varepsilon^{(\pm)}\|_{L^\infty(0,T;H^1(\Omega))}^2 + \|V_\varepsilon^{(\pm)}\|_{L^\infty(0,T;L^2(\Omega))}^2 + \rho_s \|V_\varepsilon^{(\pm)}\|_{L^2(0,T;H^1(\Omega))}^2 \\
& + \varepsilon^{-1} \|\pi^h[V_\varepsilon^+]_-\|_{L^\infty(0,T;L^2(\Omega))}^2 + \|\Psi_\varepsilon^+\|_{L^2(\Omega_T)}^2 + \varepsilon^{-1} \|\pi^h[\Psi_\varepsilon^+]_-\|_{L^2(\Omega_T)}^2 \\
& + \left\| \bar{\tau}^{\frac{1}{2}} \frac{\partial U_\varepsilon}{\partial t} \right\|_{L^2(0,T;H^1(\Omega))}^2 + \left\| \bar{\tau}^{\frac{1}{2}} \frac{\partial V_\varepsilon}{\partial t} \right\|_{L^2(\Omega_T)}^2 + \|\Xi(U_\varepsilon^+)\|^{\frac{3}{2}} \|\nabla W_\varepsilon^+\|_{L^2(\Omega_T)}^2 \\
& + \|(U_\varepsilon^+)^{\frac{1}{2}} \nabla \Psi_\varepsilon^+\|_{L^2(\Omega_T)}^2 + \left\| \mathcal{G} \frac{\partial U_\varepsilon}{\partial t} \right\|_{L^2(0,T;W^{1,q}(\Omega))}^2 + \left\| \mathcal{G} \frac{\partial V_\varepsilon}{\partial t} \right\|_{L^2(0,T;W^{1,q}(\Omega))}^2 \\
& \leq C.
\end{aligned}$$

Furthermore, we deduce from (3.2), (3.12), and (2.6) that

$$(3.13a) \quad \|U_\varepsilon - U_\varepsilon^\pm\|_{L^2(0,T;H^1(\Omega))}^2 \leq \left\| \bar{\tau} \frac{\partial U_\varepsilon}{\partial t} \right\|_{L^2(0,T;H^1(\Omega))}^2 \leq C \tau,$$

$$(3.13b) \quad \|V_\varepsilon - V_\varepsilon^\pm\|_{L^2(0,T;L^p(\Omega))}^2 \leq C h^{-d(1-\frac{2}{p})} \|V_\varepsilon - V_\varepsilon^\pm\|_{L^2(\Omega_T)}^2 \leq C h^{-d(1-\frac{2}{p})} \tau.$$

Hence on noting (3.12), (3.13a)–(3.13b), $U_\varepsilon > 0$, (1.6), assumption (iii), and a standard compact embedding result (see, e.g., [6, (1.20a)]), we can choose a subsequence $\{U_\varepsilon, W_\varepsilon^+, V_\varepsilon, \Psi_\varepsilon\}_h$ such that the convergence results (3.4a)–(3.4c), at first without the nonnegativity constraints on v and ψ , (3.5a)–(3.5d), and (3.6a)–(3.6b) for $\alpha = 1$ hold. Then (3.4a)–(3.4c) and Theorem 2.3 yield, on noting a standard compact embedding result (see, e.g., [6, (1.20b)]), assumption (i), (2.8), and (2.13), that the subsequence satisfies the additional initial and integral conditions.

The proof of the results (3.6a) for $\alpha \in (0, \infty)$, (3.7a)–(3.7b) can be found in the proof of Lemma 3.1 in BN. Furthermore, we note that Lemma 2.1 in BGN and (3.7b) imply that $\lambda(v) \geq 0$ a.e. $\Rightarrow v \geq 0$ a.e., and hence $H_{\geq 0}^1(\Omega)$ in (3.4b). Moreover, on noting that $\|[\Psi_\varepsilon^+]_-\|_{L^2(\Omega_T)} \leq \|\pi^h[\Psi_\varepsilon^+]_-\|_{L^2(\Omega_T)}$, the sixth bound in (3.12) shows that $[\Psi_\varepsilon^+]_- \rightarrow 0$ weakly in $L^2(\Omega_T)$, which implies that $[\Psi_\varepsilon^+]_+ \rightarrow \psi$ weakly in $L^2(\Omega_T)$. Hence $L_{\geq 0}^2(\Omega)$ in (3.4c), and the results (3.4d) hold on noting (1.6).

The proof, using the key entropy estimate (2.32) in the case $d = 2$, of the results (3.8)–(3.9b), the result (3.9c) if $d = 1$, and the result on U_ε in (3.9c) if $d = 2$ can be found in the proof of Lemma 3.1 in BN. To prove the result on $U_\varepsilon^\pm$ in (3.9c) for the case $d = 2$, we note the following. For any $\gamma \in (0, 1 - \frac{2}{p})$ and any $\bar{p} \in (\frac{2}{1-\gamma}, p)$ it holds on noting the compact embedding $W^{1,\bar{p}}(\Omega) \hookrightarrow C^{0,\gamma}(\bar{\Omega})$, (3.13a), and (3.9b) that

$$\begin{aligned}
(3.14) \quad & \|U_\varepsilon - U_\varepsilon^\pm\|_{L^2(0,T;C^{0,\gamma}(\bar{\Omega}))} \leq \|U_\varepsilon - U_\varepsilon^\pm\|_{L^2(0,T;W^{1,\bar{p}}(\Omega))} \\
& \leq \|U_\varepsilon - U_\varepsilon^\pm\|_{L^2(0,T;H^1(\Omega))}^\mu \|U_\varepsilon - U_\varepsilon^\pm\|_{L^2(0,T;W^{1,p}(\Omega))}^{1-\mu} \leq C \tau^{\frac{\mu}{2}},
\end{aligned}$$

where $\mu = \frac{2(p-\bar{p})}{(p-2)\bar{p}} \in (0, 1)$. Combining (3.14), assumption (iii), and the established result on U_ε in (3.9c) yields the desired result (3.9c). Then the strong convergence result (3.9c) yields the remaining results (3.9d)–(3.10c); see the proof of Lemma 3.2 in BN for details.

Finally, we have that

$$(3.15a) \quad \begin{aligned} \|\nabla(U_\varepsilon^+ - u)\|_{L^2(\Omega_T)}^2 &\leq \left| \int_{\Omega_T} \nabla(U_\varepsilon^+ - u) \cdot \nabla u \, dx \, dt \right| \\ &+ \left| \int_{\Omega_T} \nabla(U_\varepsilon^+ - \pi^h u) \cdot \nabla U_\varepsilon^+ \, dx \, dt \right| + \left| \int_{\Omega_T} \nabla(\pi^h u - u) \cdot \nabla U_\varepsilon^+ \, dx \, dt \right|, \end{aligned}$$

where, on noting (2.10),

$$(3.15b) \quad \begin{aligned} \left| \int_{\Omega_T} \nabla(U_\varepsilon^+ - \pi^h u) \cdot \nabla U_\varepsilon^+ \, dx \, dt \right| &= \left| - \int_0^T (\Delta^h U_\varepsilon^+, U_\varepsilon^+ - \pi^h u)^h \, dt \right| \\ &\leq C \|\Delta^h U_\varepsilon^+\|_{L^2(\Omega_T)} \|U_\varepsilon^+ - \pi^h u\|_{L^2(\Omega_T)}. \end{aligned}$$

Combining (3.15a)–(3.15b), (3.5a), (2.32), (2.7), (3.4a), (3.6a), and (3.13a) yields (3.11). $\square$

Remark 3.2. We remark that in the case $d = 1$ one can prove stronger versions of (3.9c)–(3.10b); see the proof of Lemma 3.1 in BN for details. We note that in BN a further time step assumption was introduced for $d = 2$, in order to prove the results (3.9c)–(3.10c). However, the proof given here shows that this assumption is not necessary; see (3.14).

Remark 3.3. One can adapt the approximation $(P_\varepsilon^{h,\tau})$ when there are no repulsive van der Waals forces ($\delta = 0$), by replacing Ξ with Ξ_ε (see Remark 3.2 in BN for details) and here in addition by replacing $U_\varepsilon^n \nabla \Psi_\varepsilon^n$ with $\pi^h[U_\varepsilon^n]_+ \nabla \Psi_\varepsilon^n$ in (2.5d). Similarly, to the insoluble surfactant system studied in BN one can now no longer guarantee the nonnegativity of U_ε . However, in contrast to the system studied in BN, it is not clear that one can prove convergence in the case $d = 1$ by adapting the techniques in BGN.

LEMMA 3.4. *Let all the assumptions of Lemma 3.1 hold, and in addition assume that if $d = 2$, then $p \in (2, 6)$, $q \in [\frac{4p}{3p-2}, 2)$, and $\tau h^{-3d(\frac{1}{2}-\frac{1}{p})} \rightarrow 0$ as $h \rightarrow 0$. Then there exists a subsequence of $\{U_\varepsilon, W_\varepsilon^+, V_\varepsilon, \Psi_\varepsilon\}_h$ such that as $h \rightarrow 0$*

$$(3.16a) \quad \mathcal{G} \frac{\partial B_\varepsilon}{\partial t} \rightarrow \mathcal{G} \frac{\partial(u \lambda(\psi))}{\partial t} \quad \text{weakly in } L^2(0, T; W^{1,q}(\Omega)),$$

$$(3.16b) \quad \Xi[U_\varepsilon^+] \Lambda_\varepsilon(\Psi_\varepsilon^+) \rightarrow u \lambda(\psi) \mathcal{I} \quad \text{strongly in } L^2(0, T; L^p(\Omega)),$$

$$(3.16c) \quad (U_\varepsilon^+)^{\frac{1}{2}} \nabla \Psi_\varepsilon^+ \rightarrow u^{\frac{1}{2}} \nabla \psi \quad \text{weakly in } L^2(\Omega_T).$$

Proof. Noting the definitions (3.1a)–(3.1b) and the bounds in (2.29a)–(2.31b) together with (2.40), (2.39) for $n = 0$, our assumption (i), (2.12), (2.13), and (2.8) imply that

$$(3.17) \quad \|B_\varepsilon^{(\pm)}\|_{L^2(0,T;W^{1,q}(\Omega))}^2 + \left\| \mathcal{G} \frac{\partial B_\varepsilon}{\partial t} \right\|_{L^2(0,T;W^{1,q}(\Omega))} \leq C$$

and hence, on noting a standard compact embedding result (see, e.g., [6, (1.20a)]), that

$$(3.18) \quad \begin{aligned} B_\varepsilon &\rightarrow b \quad \text{strongly in } L^2(0, T; L^s(\Omega)) \quad \text{as } h \rightarrow 0, \\ \mathcal{G} \frac{\partial B_\varepsilon}{\partial t} &\rightarrow \mathcal{G} \frac{\partial b}{\partial t} \quad \text{weakly in } L^2(0, T; W^{1,q}(\Omega)) \quad \text{as } h \rightarrow 0, \end{aligned}$$

where $b \in L^2(0, T; L^s(\Omega))$ still needs to be identified. Moreover, on noting (2.6), (1.25), (3.2), and (3.17), it holds for $q = p = 2$ if $d = 1$ and $q \in [\frac{4p}{3p-2}, 2)$ if $d = 2$ that

$$\begin{aligned}
 \|B_\varepsilon - B_\varepsilon^\pm\|_{L^2(0, T; L^p(\Omega))}^2 &\leq C h^{-2d(\frac{1}{2} - \frac{1}{p})} \|B_\varepsilon - B_\varepsilon^\pm\|_{L^2(0, T; L^2(\Omega))}^2 \\
 &\leq C \tau h^{-2d(\frac{1}{2} - \frac{1}{p})} \left\| \mathcal{G} \frac{\partial B_\varepsilon}{\partial t} \right\|_{L^2(0, T; W^{1, q}(\Omega))} \|B_\varepsilon^\pm\|_{L^2(0, T; W^{1, q'}(\Omega))} \\
 &\leq C \tau h^{-2d(\frac{1}{2} - \frac{1}{p})} h^{-d(\frac{1}{q} - \frac{1}{q'})} \|B_\varepsilon^\pm\|_{L^2(0, T; W^{1, q}(\Omega))} \\
 (3.19) \quad &\leq C \tau h^{-2d(\frac{1}{2} - \frac{1}{p})} h^{-d(\frac{2-q}{q})} \leq C \tau h^{-3d(\frac{1}{2} - \frac{1}{p})} \rightarrow 0 \quad \text{as } h \rightarrow 0.
 \end{aligned}$$

In addition, on noting (2.8), (1.8), and (2.6), it holds for $n = 0 \rightarrow N$ that

$$\begin{aligned}
 |B_\varepsilon^n - U_\varepsilon^n \lambda_\varepsilon(\Psi_\varepsilon^n)|_{0, p}^2 &\leq \sum_{\kappa \in T^h} [\underline{m}(\kappa)]^{\frac{2}{p}} |(I - \pi^h)[U_\varepsilon^n \lambda_\varepsilon(\Psi_\varepsilon^n)]|_{0, \infty, \kappa}^2 \\
 &\leq C \sum_{\kappa \in T^h} [\underline{m}(\kappa)]^{\frac{2}{p}} h_\kappa^2 |U_\varepsilon^n \Psi_\varepsilon^n|_{1, \infty, \kappa}^2 \leq C \sum_{\kappa \in T^h} h_\kappa^2 |U_\varepsilon^n \Psi_\varepsilon^n|_{1, p, \kappa}^2 \\
 &\leq C \sum_{\kappa \in T^h} h_\kappa^2 h_\kappa^{-2d(\frac{1}{q} - \frac{1}{p})} |U_\varepsilon^n \Psi_\varepsilon^n|_{1, q, \kappa}^2 \leq C h^{2-2d(\frac{1}{q} - \frac{1}{p})} |U_\varepsilon^n \Psi_\varepsilon^n|_{1, q}^2 \\
 (3.20) \quad &\leq C h^{2-2d(\frac{1}{q} - \frac{1}{p})} [|U_\varepsilon^n|_1^2 + |(U_\varepsilon^n)^{\frac{1}{2}}|_{0, r}^2 |(U_\varepsilon^n)^{\frac{1}{2}} \nabla \Psi_\varepsilon^n|_0^2],
 \end{aligned}$$

where $r = \infty$ if $d = 1$ and $r = \frac{2q}{2-q}$ if $d = 2$. Therefore it follows from (3.20), (3.12), and our assumptions on p and q that $\|B_\varepsilon^+ - U_\varepsilon^+ \lambda_\varepsilon(\Psi_\varepsilon^+)\|_{L^2(0, T; L^p(\Omega))} \rightarrow 0$ and hence, on noting (3.18) and (3.19), that

$$(3.21) \quad U_\varepsilon^+ \lambda_\varepsilon(\Psi_\varepsilon^+) \rightarrow b \quad \text{strongly in } L^2(0, T; L^p(\Omega)) \quad \text{as } h \rightarrow 0.$$

Combining (3.21), (3.6a), (3.9d), (3.12), and (1.8) yields, on possibly extracting a further subsequence, that $\lambda_\varepsilon(\Psi_\varepsilon^+) \rightarrow u^{-1}b$ strongly in $L^2(0, T; L^p(\Omega))$ as $h \rightarrow 0$ and in particular that $u^{-1}b \in [0, 1]$ a.e. in Ω_T . Moreover, it follows from (1.6), (1.8), (3.12), and assumption (iii) that

$$\|\lambda(\Psi_\varepsilon^+) - \lambda_\varepsilon(\Psi_\varepsilon^+)\|_{L^2(0, T; L^2(\Omega))} \leq C \varepsilon + \|[\Psi_\varepsilon^+]_-\|_{L^2(0, T; L^2(\Omega))} \leq C \varepsilon^{\frac{1}{2}} \rightarrow 0 \quad \text{as } h \rightarrow 0.$$

Hence

$$(3.22) \quad \lambda(\Psi_\varepsilon^+) \rightarrow u^{-1}b \quad \text{strongly in } L^2(0, T; L^2(\Omega)) \quad \text{as } h \rightarrow 0.$$

Combining (3.22), (1.6), and (3.5c) yields that $u^{-1}b = \psi = \lambda(\psi)$ a.e. where $u^{-1}b < 1$. It remains to identify b , where $u^{-1}b = 1$. Let $\mathcal{A} := \{(x, t) \in \Omega_T : (u^{-1}b)(x, t) = 1, \psi(x, t) < 1\}$. On assuming that $\underline{m}(\mathcal{A}) > 0$, it follows from (3.5c), (1.6), and (3.22) that

$$\begin{aligned}
 \underline{m}(\mathcal{A}) &= \int_{\Omega_T} \mathcal{H}_\mathcal{A} \, dx \, dt > \int_{\Omega_T} \psi \mathcal{H}_\mathcal{A} \, dx \, dt \leftarrow \int_{\Omega_T} \Psi_\varepsilon^+ \mathcal{H}_\mathcal{A} \, dx \, dt \\
 &\geq \int_{\Omega_T} \lambda(\Psi_\varepsilon^+) \mathcal{H}_\mathcal{A} \, dx \, dt \rightarrow \int_{\Omega_T} 1 \mathcal{H}_\mathcal{A} \, dx \, dt = \underline{m}(\mathcal{A}),
 \end{aligned}$$

where $\mathcal{H}_\mathcal{A}$ is the characteristic function of $\mathcal{A}$. This is a contradiction and hence $\underline{m}(\mathcal{A}) = 0$. This means that $\psi \geq 1$ a.e. where $u^{-1}b = 1$, i.e., $u^{-1}b = 1 = \lambda(\psi)$ a.e.

where $u^{-1}b = 1$. Combining this with the earlier result on b yields that $b = u \lambda(\psi)$ a.e. in Ω_T . This proves, on recalling (3.18), that $B_\varepsilon \rightarrow u \lambda(\psi)$ strongly in $L^2(0, T; L^s(\Omega))$ as $h \rightarrow 0$, and that (3.16a) holds.

Similarly to (3.20), we have on noting Lemma 2.1 in BGN, Lemma 2.3 in BN, and (3.7a) that

$$\begin{aligned} & \|U_\varepsilon^+ \lambda_\varepsilon(\Psi_\varepsilon^+) \mathcal{I} - \Xi(U_\varepsilon^+) \Lambda_\varepsilon(\Psi_\varepsilon^+)\|_{L^2(0, T; L^p(\Omega))}^2 \\ & \leq \|U_\varepsilon^+ [\lambda_\varepsilon(\Psi_\varepsilon^+) \mathcal{I} - \Lambda_\varepsilon(\Psi_\varepsilon^+)]\|_{L^2(0, T; L^p(\Omega))}^2 + \|[U_\varepsilon^+ \mathcal{I} - \Xi(U_\varepsilon^+)] \Lambda_\varepsilon(\Psi_\varepsilon^+)\|_{L^2(0, T; L^p(\Omega))}^2 \\ & \leq \int_0^T \sum_{\kappa \in \mathcal{T}^h} h_\kappa^2 |U_\varepsilon^+ \nabla \Psi_\varepsilon^+|_{0, p, \kappa}^2 dt + \|U_\varepsilon^+ \mathcal{I} - \Xi(U_\varepsilon^+)\|_{L^2(0, T; L^p(\Omega))}^2 \rightarrow 0 \text{ as } h \rightarrow 0. \end{aligned}$$

Combining this and (3.21) yields the desired result (3.16b).

Finally, it follows from (3.12) that $(U_\varepsilon^+)^{\frac{1}{2}} \nabla \Psi_\varepsilon^+ \rightarrow z$ weakly in $L^2(\Omega_T)$, where $z \in L^2(\Omega_T)$. But for any $\eta \in C_0^\infty(\overline{\Omega_T})$, which is dense in $L^2(\Omega_T)$, we have, on recalling (3.6a), (3.5c), and (3.11), that

$$\begin{aligned} & \int_0^T (u^{\frac{1}{2}} z, \eta) dt \leftarrow \int_0^T (U_\varepsilon^+ \nabla \Psi_\varepsilon^+, \eta) dt = - \int_0^T [(\Psi_\varepsilon^+ \nabla U_\varepsilon^+, \eta) + (\Psi_\varepsilon^+ U_\varepsilon^+, \nabla \cdot \eta)] dt \\ (3.23) \quad & \rightarrow - \int_0^T (\psi \nabla u, \eta) dt - \int_0^T (\psi u, \nabla \cdot \eta) dt = \int_0^T (u \nabla \psi, \eta) dt. \end{aligned}$$

Hence $z = u^{\frac{1}{2}} \nabla \psi$ in $L^2(\Omega_T)$ and (3.16c) holds. $\square$

THEOREM 3.5. *Let all the assumptions of Lemma 3.4 hold. Then there exist a subsequence of $\{U_\varepsilon, W_\varepsilon^+, V_\varepsilon, \Psi_\varepsilon\}_h$, where $\{U_\varepsilon, W_\varepsilon^+, V_\varepsilon, \Psi_\varepsilon\}$ solve $(P_\varepsilon^{h, \tau})$, and functions $\{u, w, v, \psi\}$ satisfying (3.4a)–(3.4d), (3.8), and (3.9d). In addition, as $h \rightarrow 0$ the following hold: (3.5a)–(3.5d), (3.6a)–(3.6b), (3.7a)–(3.7b), (3.9a)–(3.9c), (3.10a)–(3.10b) for a.a. $t \in (0, T)$, (3.10c), (3.11), and (3.16a)–(3.16c). Moreover, we have that u and v fulfill $u(\cdot, 0) = u^0(\cdot)$ in Y_1 , $v(\cdot, 0) = v^0(\cdot)$ in Y_2 , where $H^1(\Omega) \xhookrightarrow{c} Y_1$, $L^2(\Omega) \xhookrightarrow{c} Y_2$. Furthermore, $\{u, w, v, \psi\}$ satisfy for all $\eta \in L^2(0, T; W^{1, q'}(\Omega))$, with $q' = 2$ if $d = 1$ and $q' \in (2, \frac{4p}{p+2}]$, where $p \in (2, 6)$, if $d = 2$,*

$$(3.24a) \quad \int_0^T \left\langle \frac{\partial u}{\partial t}, \eta \right\rangle_{q'} dt + \int_{\Omega_T} \left[\frac{1}{3} u^3 \nabla w \cdot \nabla \eta + \frac{1}{2} u^2 \nabla v \cdot \nabla \eta \right] dx dt = 0,$$

$$(3.24b) \quad \begin{aligned} & \int_0^T \left\langle \frac{\partial v}{\partial t}, \eta \right\rangle_{q'} dt + \int_{\Omega_T} [\rho_s \nabla v \cdot \nabla \eta + u \lambda(v) \nabla v \cdot \nabla \eta] dx dt \\ & + \int_{\Omega_T} \left[\frac{1}{2} u^2 \lambda(v) \nabla w \cdot \nabla \eta - K(\psi - v) \eta \right] dx dt = 0, \end{aligned}$$

$$(3.24c) \quad \begin{aligned} & \int_0^T \left\langle \frac{\partial(u \lambda(\psi))}{\partial t}, \eta \right\rangle_{q'} dt + \int_{\Omega_T} \left[\rho_b u \nabla \psi \cdot \nabla \eta + \frac{1}{3} u^3 \lambda(\psi) \nabla w \cdot \nabla \eta \right] dx dt \\ & + \int_{\Omega_T} \left[\frac{1}{2} u^2 \lambda(\psi) \nabla v \cdot \nabla \eta + \beta K(\psi - v) \eta \right] dx dt = 0, \end{aligned}$$

where for a.a. $t \in (0, T)$

$$(3.24d) \quad \int_{\Omega} [w(\cdot, t) \xi - c \nabla u(\cdot, t) \cdot \nabla \xi - \phi(u(\cdot, t)) \xi] dx = 0 \quad \forall \xi \in H^1(\Omega).$$

Proof. On choosing $z^h \equiv \pi^h \tilde{\xi}$, where $\tilde{\xi} \in W^{1,p}(\Omega)$, in (3.3d); it follows from (2.1), (2.10), (2.7), (3.5a), and (3.10a)–(3.10b) that (3.24d) holds for $\xi \equiv \tilde{\xi}$. The desired result (3.24d) then holds for any $\xi \in H^1(\Omega)$ via a density argument.

For any $\eta \in L^2(0, T; W^{1,q'}(\Omega))$ and $\tilde{\eta} \in H^1(0, T; W^{1,\infty}(\Omega))$, we choose $\chi \equiv \pi^h \eta$ in (3.3a)–(3.3c) and then analyze the subsequent terms. The results (3.24a) and (3.24b), for the case $K = 0$, are then derived from (3.3a) and (3.3b), with $K = 0$; their proof can be found in the proof of Theorem 3.1 in BN. Hence it is sufficient to prove (3.24c), as the convergence of the term involving K in (3.24b) then follows from the convergence of the corresponding term in (3.24c).

First, (2.11), (2.15), an interpolation estimate in time (see [6, (1.19)]), (3.12), (3.17), and (2.8), on noting that $\|B_\varepsilon\|_{L^\infty(0,T;L^2(\Omega))} \leq \|U_\varepsilon\|_{L^\infty(0,T;L^2(\Omega))}$, yield that

$$\begin{aligned}
 (3.25) \quad & \left| \int_0^T \left[\left(\frac{\partial B_\varepsilon}{\partial t}, \pi^h \eta \right)^h - \left(\frac{\partial B_\varepsilon}{\partial t}, \pi^h \tilde{\eta} \right) \right] dt \right| \\
 & \leq \left| \int_0^T \left[\left(\frac{\partial B_\varepsilon}{\partial t}, \pi^h [\eta - \tilde{\eta}] \right)^h - \left(\frac{\partial B_\varepsilon}{\partial t}, \pi^h [\eta - \tilde{\eta}] \right) \right] dt \right| \\
 & \quad + \left| - \int_0^T \left(B_\varepsilon, \frac{\partial(\pi^h \tilde{\eta})}{\partial t} \right)^h dt + (B_\varepsilon(\cdot, T), \pi^h \tilde{\eta}(\cdot, T))^h - (B_\varepsilon(\cdot, 0), \pi^h \tilde{\eta}(\cdot, 0))^h \right. \\
 & \quad \left. + \int_0^T \left(B_\varepsilon, \frac{\partial(\pi^h \tilde{\eta})}{\partial t} \right) dt - (B_\varepsilon(\cdot, T), \pi^h \tilde{\eta}(\cdot, T)) + (B_\varepsilon(\cdot, 0), \pi^h \tilde{\eta}(\cdot, 0)) \right| \\
 & \leq C \left\| \mathcal{G} \frac{\partial B_\varepsilon}{\partial t} \right\|_{L^2(0,T;W^{1,q}(\Omega))} \|\pi^h [\eta - \tilde{\eta}]\|_{L^2(0,T;W^{1,q'}(\Omega))} \\
 & \quad + C h \|B_\varepsilon\|_{L^\infty(0,T;L^2(\Omega))} \|\pi^h \tilde{\eta}\|_{H^1(0,T;H^1(\Omega))} \\
 & \leq C \|\eta - \tilde{\eta}\|_{L^2(0,T;W^{1,q'}(\Omega))} + C h \|\tilde{\eta}\|_{H^1(0,T;W^{1,q'}(\Omega))}.
 \end{aligned}$$

Furthermore, it follows from (1.25) and (3.17) that

$$\begin{aligned}
 (3.26) \quad & \left| \int_0^T \left(\frac{\partial B_\varepsilon}{\partial t}, (I - \pi^h) \eta \right) dt \right| \leq C \left\| \mathcal{G} \frac{\partial B_\varepsilon}{\partial t} \right\|_{L^2(0,T;W^{1,q}(\Omega))} \|(I - \pi^h) \eta\|_{L^2(0,T;W^{1,q'}(\Omega))} \\
 & \leq C \|(I - \pi^h) \eta\|_{L^2(0,T;W^{1,q'}(\Omega))}.
 \end{aligned}$$

Combining (3.25), the denseness of $H^1(0, T; W^{1,\infty}(\Omega))$ in $L^2(0, T; W^{1,q'}(\Omega))$, (3.26), (2.7), (1.25), and (3.16a) yields for all $\eta \in L^2(0, T; W^{1,q'}(\Omega))$ that

$$(3.27) \quad \int_0^T \left(\frac{\partial B_\varepsilon}{\partial t}, \pi^h \eta \right)^h dt \rightarrow \int_0^T \left\langle \frac{\partial(u \lambda(\psi))}{\partial t}, \eta \right\rangle_{q'} dt \quad \text{as } h \rightarrow 0.$$

Similarly to the above, it follows from (2.1), (2.11), (2.8), (3.5b), and (3.5c) that for all $\eta \in L^2(0, T; W^{1,q'}(\Omega))$

$$(3.28) \quad \int_0^T (\Psi_\varepsilon^+ - V_\varepsilon^+, \pi^h \eta)^h dt \rightarrow \int_0^T (\psi - v, \eta) dt \quad \text{as } h \rightarrow 0.$$

In view of (3.12), (3.4a), [6, (1.19)], and (3.16c), we deduce with r as defined in

(2.31a) that for all $\eta \in L^2(0, T; W^{1,q'}(\Omega))$ and for all $\tilde{\eta} \in H^1(0, T; W^{1,\infty}(\Omega))$

$$\begin{aligned}
 & \left| \int_0^T (U_\varepsilon^+ \nabla \Psi_\varepsilon^+, \nabla[\tilde{\eta} - \pi^h \eta]) \, dt \right| + \left| \int_0^T (u \nabla \psi, \nabla[\tilde{\eta} - \eta]) \, dt \right| \\
 & \leq \| (U_\varepsilon^+)^{\frac{1}{2}} \|_{L^\infty(0,T;L^r(\Omega))} \| (U_\varepsilon^+)^{\frac{1}{2}} \nabla \Psi_\varepsilon^+ \|_{L^2(\Omega_T)} \| \tilde{\eta} - \pi^h \eta \|_{L^2(0,T;W^{1,q'}(\Omega))} \\
 & \quad + \| u^{\frac{1}{2}} \|_{L^\infty(0,T;L^r(\Omega))} \| u^{\frac{1}{2}} \nabla \psi \|_{L^2(\Omega_T)} \| \tilde{\eta} - \eta \|_{L^2(0,T;W^{1,q'}(\Omega))} \\
 (3.29) \quad & \leq C [\| (I - \pi^h) \eta \|_{L^2(0,T;W^{1,q'}(\Omega))} + \| \eta - \tilde{\eta} \|_{L^2(0,T;W^{1,q'}(\Omega))}].
 \end{aligned}$$

Similarly to the above, on noting in addition (2.31b), Lemma 2.1 in BGN, (3.10c), (3.4d), and (3.4b), we deduce for all $\eta \in L^2(0, T; W^{1,q'}(\Omega))$ and for all $\tilde{\eta} \in H^1(0, T; W^{1,\infty}(\Omega))$

$$\begin{aligned}
 & \left| \int_0^T ([\Xi(U_\varepsilon^+)]^3 \Lambda_\varepsilon(\Psi_\varepsilon^+) \nabla W_\varepsilon^+, \nabla[\tilde{\eta} - \pi^h \eta]) \, dt \right| + \left| \int_0^T (u^3 \lambda(\psi) \nabla w, \nabla[\tilde{\eta} - \eta]) \, dt \right| \\
 & \leq \| [\Xi(U_\varepsilon^+)]^{\frac{3}{2}} \|_{L^\infty(0,T;L^r(\Omega))} \| [\Xi(U_\varepsilon^+)]^{\frac{3}{2}} \nabla W_\varepsilon^+ \|_{L^2(\Omega_T)} \| \tilde{\eta} - \pi^h \eta \|_{L^2(0,T;W^{1,q'}(\Omega))} \\
 & \quad + \| \lambda(\psi) \|_{L^\infty(\Omega_T)} \| u^{\frac{3}{2}} \|_{L^\infty(0,T;L^r(\Omega))} \| u^{\frac{3}{2}} \nabla w \|_{L^2(\Omega_T)} \| \tilde{\eta} - \eta \|_{L^2(0,T;W^{1,q'}(\Omega))} \\
 & \leq C [\| (I - \pi^h) \eta \|_{L^2(0,T;W^{1,q'}(\Omega))} + \| \eta - \tilde{\eta} \|_{L^2(0,T;W^{1,q'}(\Omega))}]
 \end{aligned}$$

and

$$\begin{aligned}
 & \left| \int_0^T ([\Xi(U_\varepsilon^+)]^{\frac{3}{2}} [\Xi(U_\varepsilon^-)]^{\frac{1}{2}} \Lambda_\varepsilon(\Psi_\varepsilon^+) \nabla V_\varepsilon^-, \nabla[\tilde{\eta} - \pi^h \eta]) \, dt \right| \\
 & \quad + \left| \int_0^T (u^2 \lambda(\psi) \nabla v, \nabla[\tilde{\eta} - \eta]) \, dt \right| \\
 & \leq \| [\Xi(U_\varepsilon^+)]^{\frac{3}{2}} [\Xi(U_\varepsilon^-)]^{\frac{1}{2}} \|_{L^\infty(0,T;L^r(\Omega))} \| \nabla V_\varepsilon^- \|_{L^2(\Omega_T)} \| \tilde{\eta} - \pi^h \eta \|_{L^2(0,T;W^{1,q'}(\Omega))} \\
 & \quad + \| \lambda(\psi) \|_{L^\infty(\Omega_T)} \| u^2 \|_{L^\infty(0,T;L^r(\Omega))} \| \nabla v \|_{L^2(\Omega_T)} \| \tilde{\eta} - \eta \|_{L^2(0,T;W^{1,q'}(\Omega))} \\
 (3.30) \quad & \leq C [\| (I - \pi^h) \eta \|_{L^2(0,T;W^{1,q'}(\Omega))} + \| \eta - \tilde{\eta} \|_{L^2(0,T;W^{1,q'}(\Omega))}].
 \end{aligned}$$

For all $\tilde{\eta} \in H^1(0, T; W^{1,\infty}(\Omega))$, it follows from (3.6a), (3.16c), (3.7a), (3.16b), (3.10c), (3.4a), (3.4d), [6, (1.19)], (2.31b), (3.1b), (3.12), and (3.5b) that as $h \rightarrow 0$

$$(3.31a) \quad \int_{\Omega_T} (U_\varepsilon^+)^{\frac{1}{2}} [(U_\varepsilon^+)^{\frac{1}{2}} \nabla \Psi_\varepsilon^+] \nabla \tilde{\eta} \, dx \, dt \rightarrow \int_{\Omega_T} u^{\frac{1}{2}} [u^{\frac{1}{2}} \nabla \psi] \nabla \tilde{\eta} \, dx \, dt,$$

$$\begin{aligned}
 & \int_{\Omega_T} [\Xi(U_\varepsilon^+)]^{\frac{1}{2}} [\Xi(U_\varepsilon^+) \Lambda_\varepsilon(\Psi_\varepsilon^+)] [\Xi(U_\varepsilon^+)]^{\frac{3}{2}} \nabla W_\varepsilon^+ \nabla \tilde{\eta} \, dx \, dt \\
 (3.31b) \quad & \rightarrow \int_{\Omega_T} u^{\frac{1}{2}} [u \lambda(\psi)] [u^{\frac{3}{2}} \nabla w] \nabla \tilde{\eta} \, dx \, dt,
 \end{aligned}$$

$$\begin{aligned}
 & \int_{\Omega} [\Xi(U_\varepsilon^+)]^{\frac{1}{2}} [\Xi(U_\varepsilon^-)]^{\frac{1}{2}} [\Xi(U_\varepsilon^+) \Lambda_\varepsilon(\Psi_\varepsilon^+)] \nabla V_\varepsilon^- \nabla \tilde{\eta} \, dx \, dt \\
 (3.31c) \quad & \rightarrow \int_{\Omega_T} u [u \lambda(\psi)] \nabla v \nabla \tilde{\eta} \, dx \, dt.
 \end{aligned}$$

Noting that $H^1(0, T; W^{1,\infty}(\Omega))$ is dense in $L^2(0, T; W^{1,q'}(\Omega))$ and (2.7), we obtain the desired result (3.24c) on combining (3.3c), (3.27)–(3.30), and (3.31a)–(3.31c). Hence $\{u, w, v, \psi\}$ satisfy (3.24a)–(3.24d) as well as the stated results of Lemmas 3.1 and 3.4. $\square$

4. Numerical results. Before presenting some numerical results in both one and two space dimensions, we briefly state algorithms for solving the resulting system of algebraic equations for $\{U_\varepsilon^n, W_\varepsilon^n, V_\varepsilon^n, \Psi_\varepsilon^n\}$ arising at each time level from the approximation $(P_\varepsilon^{h,\tau})$. As (2.5a)–(2.5b) in $(P_\varepsilon^{h,\tau})$ are independent of $\{V_\varepsilon^n, \Psi_\varepsilon^n\}$, we first solve these to obtain $\{U_\varepsilon^n, W_\varepsilon^n\}$; then we solve (2.5c)–(2.5d) for $\{V_\varepsilon^n, \Psi_\varepsilon^n\}$. We use the following iterative approach to solve (2.5a)–(2.5b) for $\{U_\varepsilon^n, W_\varepsilon^n\}$: Given $U_\varepsilon^{n,0} \in S_{>0}^h$, for $k \geq 1$ find $\{U_\varepsilon^{n,k}, W_\varepsilon^{n,k}\} \in [S^h]^2$ such that for all $\chi \in S^h$

$$(4.1a) \quad \left(\frac{U_\varepsilon^{n,k} - U_\varepsilon^{n-1}}{\tau_n}, \chi \right)^h + \frac{1}{3} ([\Xi(U_\varepsilon^{n,k-1})]^3 \nabla W_\varepsilon^{n,k}, \nabla \chi) \\ = -\frac{1}{2} ([\Xi(U_\varepsilon^{n,k-1})]^{\frac{3}{2}} [\Xi(U_\varepsilon^{n-1})]^{\frac{1}{2}} \nabla V_\varepsilon^{n-1}, \nabla \chi),$$

$$(4.1b) \quad c(\nabla U_\varepsilon^{n,k}, \nabla \chi) + (\phi^+(U_\varepsilon^{n,k}) + \phi^-(U_\varepsilon^{n-1}), \chi)^h = (W_\varepsilon^{n,k}, \chi)^h.$$

Then, having obtained $\{U_\varepsilon^n, W_\varepsilon^n\}$, we solve (2.5c)–(2.5d) for $\{V_\varepsilon^n, \Psi_\varepsilon^n\}$ using the following iterative approach: Given $\{V_\varepsilon^{n,0}, \Psi_\varepsilon^{n,0}\} \in [S^h]^2$, for $k \geq 1$ find $\{V_\varepsilon^{n,k}, \Psi_\varepsilon^{n,k}\} \in [S^h]^2$ such that for all $\chi \in S^h$

$$(4.2a) \quad \left(\frac{V_\varepsilon^{n,k} - V_\varepsilon^{n-1}}{\tau_n}, \chi \right)^h + \rho_s (\nabla V_\varepsilon^{n,k}, \nabla \chi) + (\Xi(U_\varepsilon^n) \Lambda_\varepsilon(V_\varepsilon^{n,k-1}) \nabla V_\varepsilon^{n,k}, \nabla \chi) \\ - K (\Psi_\varepsilon^{n,k-1} - V_\varepsilon^{n,k}, \chi)^h = -\frac{1}{2} ([\Xi(U_\varepsilon^n)]^2 \Lambda_\varepsilon(V_\varepsilon^{n,k-1}) \nabla W_\varepsilon^n, \nabla \chi),$$

$$(4.2b) \quad \left(\frac{U_\varepsilon^n \lambda_\varepsilon(\Psi_\varepsilon^{n,k}) - U_\varepsilon^{n-1} \lambda_\varepsilon(\Psi_\varepsilon^{n-1})}{\tau_n}, \chi \right)^h + \rho_b (U_\varepsilon^n \nabla \Psi_\varepsilon^{n,k}, \nabla \chi) \\ + \frac{1}{3} ([\Xi(U_\varepsilon^n)]^3 \Lambda_\varepsilon(\Psi_\varepsilon^{n,k-1}) \nabla W_\varepsilon^n, \nabla \chi) + \beta K (\Psi_\varepsilon^{n,k} - V_\varepsilon^{n,k}, \chi)^h \\ = -\frac{1}{2} ([\Xi(U_\varepsilon^n)]^{\frac{3}{2}} [\Xi(U_\varepsilon^{n-1})]^{\frac{1}{2}} \Lambda_\varepsilon(\Psi_\varepsilon^{n,k-1}) \nabla V_\varepsilon^{n-1}, \nabla \chi).$$

Equations (4.1a)–(4.1b) and (4.2a)–(4.2b) are natural extensions of the iterative procedure proposed in [10] for solving a finite element approximation of the thin film equation. Note that we have chosen the iterative method such that (4.2a) and (4.2b) decouple. As $U_\varepsilon^{n,k-1} > 0$, it is easily established on noting Lemma 2.2 in BN that there exists a unique solution $\{U_\varepsilon^{n,k}, W_\varepsilon^{n,k}\} \in S_{>0}^h \times S^h$ to (4.1a)–(4.1b). As (4.2a) is linear, existence of $V_\varepsilon^{n,k}$ follows from uniqueness; this is easily established on noting (2.2a) and $\rho_s \geq 0$. Existence and uniqueness of $\Psi_\varepsilon^{n,k}$ follow from the monotonicity of λ_ε and the positivity of $U_\varepsilon^n > 0$. Hence the iterations (4.1a)–(4.1b) and (4.2a)–(4.2b) are well defined.

For the iterative algorithms (4.1a)–(4.1b) and (4.2a)–(4.2b) we set, for $n \geq 1$, $\{U_\varepsilon^{n,0}, V_\varepsilon^{n,0}, \Psi_\varepsilon^{n,0}\} \equiv \{U_\varepsilon^{n-1}, V_\varepsilon^{n-1}, \Psi_\varepsilon^{n-1}\}$ and adopted the stopping criteria

$$|U_\varepsilon^{n,k} - U_\varepsilon^{n,k-1}|_{0,\infty} < tol, \quad |V_\varepsilon^{n,k} - V_\varepsilon^{n,k-1}|_{0,\infty} < tol, \quad \text{and} \quad |\Psi_\varepsilon^{n,k} - \Psi_\varepsilon^{n,k-1}|_{0,\infty} < tol,$$

respectively, with $tol = 10^{-8}$. Furthermore, we then set $\{U_\varepsilon^n, W_\varepsilon^n, V_\varepsilon^n, \Psi_\varepsilon^n\} \equiv \{U_\varepsilon^{n,k}, W_\varepsilon^{n,k}, V_\varepsilon^{n,k}, \Psi_\varepsilon^{n,k}\}$ for (4.1a)–(4.1b) and (4.2a)–(4.2b).

Remark 4.1. The nonlinear system (4.1a)–(4.1b) can be solved using an inexact Newton's method, applying a BiCGSTAB algorithm at each Newton iteration. The linear system (4.2a), on the other hand, can be solved efficiently using a conjugate

gradient algorithm. The nonlinear system (4.2b) can be solved with a nonlinear SOR method, similar to the one employed in [7]. In particular, in each step and at each vertex a scalar nonlinear equation of the form $\alpha_1 \lambda_\varepsilon(s) + \alpha_2 s = \alpha_3$, $s \in \mathbb{R}$, where $\alpha_1, \alpha_2 > 0$, has to be solved, which is straightforward as λ_ε is monotone.

Although we are unable to show convergence of the iterations (4.1a)–(4.1b) and (4.2a)–(4.2b) for $\{U_\varepsilon^n, W_\varepsilon^n\}$ and $\{V_\varepsilon^n, \Psi_\varepsilon^n\}$, respectively, we observed good convergence properties in practice.

4.1. Numerical results for $d = 1$. First, we present numerical experiments in one space dimension. Throughout we choose a uniform partitioning of $\Omega = (-L, L)$, where $L \geq 1$, with mesh points $p_j = -L + (j-1)h$, $j = 1 \rightarrow 2^{10} + 1$, where $h = 2^{-9} L$. In addition we choose uniform time steps $\tau_n = \tau = 10^{-3}$ and throughout set the regularization parameter $\varepsilon = 10^{-5}$. For the initial profiles u^0 , v^0 , and ψ^0 , we set

$$(4.3) \quad u^0(x) = 1 \quad \text{and} \quad v^0(x) = \frac{1}{2} [1 - \tanh(10|x| - 5)], \quad \psi^0(x) = 0,$$

which resembles a uniform liquid film of unit height with surfactant on top of it, and the film is uncontaminated by the chemical. In the absence of both surfactant and chemical, a uniform film is a steady state. We choose $U_\varepsilon^0 \equiv \pi^h u^0$, $V_\varepsilon^0 \equiv \pi^h v^0$, and $\Psi_\varepsilon^0 \equiv \pi^h \psi^0$ as the discrete initial data on noting that $u^0, v^0, \psi^0 \in W^{1,\infty}(\Omega)$.

We now report on the evolutions of U_ε , V_ε , and Ψ_ε for similar parameters as in some of the experiments in [16, Fig. 5]. We set $L = 10$, $c = 10^{-3}$, $\rho_s = 10^{-5}$, $\rho_b = 10^{-2}$, $K = 1$, $a = 0$, $\delta = 10^{-5}$, and $\nu = 4$ and used the initial data (4.3). We then varied the solubility parameter, by choosing $\beta = 0.01, 1$, or 100 . The different evolution results can be seen in Figure 1, where we plot U_ε and V_ε both at time $t = 5$ and at different final times T . Note that for brevity only V_ε is displayed since in all cases after a short time Ψ_ε is graphically indistinguishable from it. This is to be expected from the Lyapunov structure (2.29a) (see also (1.20)) on noting (1.11) and (1.8).

One can clearly see the effect of the parameter β on the evolution. On the one hand, the larger the value of β the faster Ψ_ε attains the profile of V_ε . On the other hand, since the quantity $f(V_\varepsilon^n + \frac{1}{\beta} \pi^h [U_\varepsilon^n \lambda_\varepsilon(\Psi_\varepsilon^n)]) = f(V_\varepsilon^0 + \frac{\varepsilon}{\beta})$ is preserved, the value of β dictates how much surfactant material V_ε remains on the film surface. In particular, after a sufficiently long time it holds that $f V_\varepsilon^n \approx f \Psi_\varepsilon^n$ and $f(V_\varepsilon^n + \frac{1}{\beta} \pi^h [U_\varepsilon^n V_\varepsilon^n]) \approx f V_\varepsilon^0$. Hence if β is such that $\varepsilon \ll \beta \ll 1$, the original drop of surfactant almost completely disappears, leading to a comparatively small change in the liquid film height that quickly smooths out. In the case of a very large β , recall that $\beta \rightarrow \infty$ models insoluble surfactant spreading; the initial amount of surfactant is almost completely preserved, leading to a fast propagating wave front.

Finally, note that the presence of repulsive van der Waals forces ($\delta > 0$) has no effect on the evolution in this case, as the film height is always bounded well away from zero.

When attractive van der Waals forces are included, however, this has a marked effect on the film evolution. We repeated the above experiments for a value of $a = 5 \times 10^{-4}$, and the results can be seen in Figure 2. Note that for $\beta = 0.01$ and 1 the film has thinned considerably in some areas due to the presence of attractive van der Waals forces, although it can never actually rupture ($U_\varepsilon = 0$) due to the repulsive van der Waals forces, ϕ^+ . In fact, it holds that $\min_{x \in \bar{\Omega}} U_\varepsilon(x, T) = \arg \min_{s \in \mathbb{R}_{>0}} \Phi(s) = (\frac{\delta}{a})^{\frac{1}{\nu-3}} = 0.02$. For $\beta = 100$, on the other hand, the film has not yet completely thinned at the displayed time.

FIG. 1. $U_\varepsilon(x, t)$ and $V_\varepsilon(x, t)$ for $\beta \in \{0.01, 1, 100\}$ and time $t = 5$ (above), and for different final times $t = T$ (below).

FIG. 2. $U_\varepsilon(x, T)$ and $V_\varepsilon(x, T)$ for $\beta \in \{0.01, 1, 100\}$ for different final times T .

FIG. 3. $U_\varepsilon(x, T)$ for $\beta = 0.01, T = 5$ (left), for $\beta = 1, T = 3$ (middle), and for $\beta = 100, T = 2$ (right).

FIG. 4. $U_\varepsilon(x, T)$ and $V_\varepsilon(x, T)$ for $\beta = 0.01$ and $T = 1$. On the right a plot of $U_\varepsilon(x, T)|_{x_2=0}$ and $V_\varepsilon(x, T)|_{x_2=0}$.

4.2. Numerical results for $d = 2$. Finally, we present a numerical experiment in two space dimensions with $\Omega = (-L, L) \times (-L, L)$. We took a uniform mesh of squares of length $h = \frac{2L}{128}$, each of which was divided into two triangles by its northeast diagonal. We chose the following parameters for $(P_\varepsilon^{h,\tau})$: $L = 2.5$, $c = 10^{-3}$, $\rho_s = 10^{-5}$, $\rho_b = 10^{-2}$, $K = 1$, $a = 0$, $\delta = 10^{-5}$, $\nu = 7$, $\tau_n = \tau = 10^{-3}$, and $\varepsilon = 10^{-5}$. For the initial profiles we chose (4.3). We set $U_\varepsilon^0 \equiv \pi^h u^0$, $V_\varepsilon^0 \equiv \pi^h v^0$, and $\Psi_\varepsilon \equiv \pi^h \psi^0$. In Figure 3 we plot $U_\varepsilon(x, T)$ for $\beta = 0.01, 1$, and 100 at different final times T .

Though on a slower time scale, the results are qualitatively similar to the experiments in one space dimension. The same holds true when including attractive van der Waals forces in the simulation. See Figure 4, where we plot U_ε and V_ε for $\beta = 0.01$ and the same parameters as above except $a = 0.02$. Again for brevity only V_ε is displayed since Ψ_ε is graphically indistinguishable from it. Note that here $\min_{x \in \bar{\Omega}} U_\varepsilon(x, T) \approx \arg \min_{s \in \mathbb{R}_{>0}} \Phi(s) = (\frac{\delta}{a})^{\frac{1}{\nu-3}} \approx 0.15$.

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