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Abstract

In this paper, we analyze a general diffuse interface model for incompressible two-phase flows with unmatched densities in a smooth bounded domain $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$). This model describes the evolution of free interfaces in contact with the solid boundary, that is, the moving contact lines. The corresponding evolution system consists of a nonhomogeneous Navier–Stokes equation for the (volume) averaged fluid velocity $\mathbf{v}$ that is nonlinearly coupled with a convective Cahn–Hilliard equation for the order parameter φ. Due to the nontrivial boundary dynamics, the fluid velocity satisfies a generalized Navier boundary condition that accounts for the velocity slippage and uncompensated Young stresses at the solid boundary, while the order parameter fulfils a dynamic boundary condition with surface convection. We prove the existence of a global weak solution for arbitrary initial data in both two and three dimensions. The proof relies on a combination of suitable approximations and regularizations of the original system together with a novel time-implicit discretization scheme based on the energy dissipation law.

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Global Weak Solutions to a Diffuse Interface Model for Incompressible Two-Phase Flows with Moving Contact Lines and Different Densities

Ciprian G. Gal, Maurizio Grasselli & Hao Wu

Communicated by F. Lin

Abstract

In this paper, we analyze a general diffuse interface model for incompressible two-phase flows with unmatched densities in a smooth bounded domain $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$). This model describes the evolution of free interfaces in contact with the solid boundary, that is, the moving contact lines. The corresponding evolution system consists of a nonhomogeneous Navier–Stokes equation for the (volume) averaged fluid velocity $\mathbf{v}$ that is nonlinearly coupled with a convective Cahn–Hilliard equation for the order parameter φ. Due to the nontrivial boundary dynamics, the fluid velocity satisfies a generalized Navier boundary condition that accounts for the velocity slippage and uncompensated Young stresses at the solid boundary, while the order parameter fulfils a dynamic boundary condition with surface convection. We prove the existence of a global weak solution for arbitrary initial data in both two and three dimensions. The proof relies on a combination of suitable approximations and regularizations of the original system together with a novel time-implicit discretization scheme based on the energy dissipation law. 1

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1. Introduction

In immiscible two-phase flows the contact line is defined as the intersection of the fluid–fluid interface with the solid wall. The contact line problem turns out to be of critical importance in many applications such as microfluidics, inkjet printing, coating and oil recovery (see for example, [13,24,27,54]). The (static) contact angle along the contact line characterizes fundamental concepts of wetting and spreading phenomena on the solid surface (see Fig. 1). Furthermore, when one fluid displaces another immiscible fluid, the contact line is moving relative to the solid wall, resulting in a dynamic contact angle which deviates from the static one. It is well-known that in immiscible two-phase flows, the moving contact line (MCL) is incompatible with the no-slip boundary condition and predicts a non-integrable singularity for the viscous stress, which results in a non-physical divergence for the energy dissipation rate [27,28,43]. Much effort has been made to remove the singularity, and various continuum models were proposed to regularize the problem, see for instance [27,39,60–62] and the references cited therein. Among those contributions, the diffuse interface model turns out to be a useful and attractive method to resolve the MCL conundrum [25,41,45,57,59,65,69,70,73]. The diffuse interface models replace the classical hypersurface description of the free interface between two fluids (that is, the so-called sharp interface) with a thin interfacial layer where microscopic mixing of the macroscopically distinct components of matter are allowed, so that possible topological transitions such as pinch off and reconnection of fluid interfaces can be handled in a natural way (see for example, [8,49]). Moreover, the corresponding nonlinear partial differential equations satisfy certain natural thermodynamics consistent energy dissipation laws, which make it possible to carry out further mathematical analysis [19,34,48] and design efficient energy stable numerical schemes [9,22,36,64].

In this paper, we consider a thermodynamically consistent diffuse interface model for an incompressible two-phase flow with different densities in a bounded domain $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$) that accounts for the dynamics of moving contact lines on the boundary $\partial\Omega$. The resulting evolution system is of Cahn–Hilliard–Navier–Stokes type:

$$\begin{cases} \partial_t(\rho\mathbf{v}) + \mathrm{div}(\rho\mathbf{v}\otimes\mathbf{v}) - \mathrm{div}(2\nu(\varphi)D\mathbf{v}) + \nabla p & \\ \qquad + \mathrm{div}(\mathbf{v}\otimes\mathbf{J}) = \mu\nabla\varphi, & \text{in } Q_\infty,\\ \mathrm{div}\,\mathbf{v} = 0, & \text{in } Q_\infty,\\ \partial_t\varphi + \mathbf{v}\cdot\nabla\varphi = \mathrm{div}\left(m(\varphi)\nabla\mu\right), & \text{in } Q_\infty,\\ \mu = -\Delta\varphi + f(\varphi), & \text{in } Q_\infty, \end{cases} \tag{1.1}$$

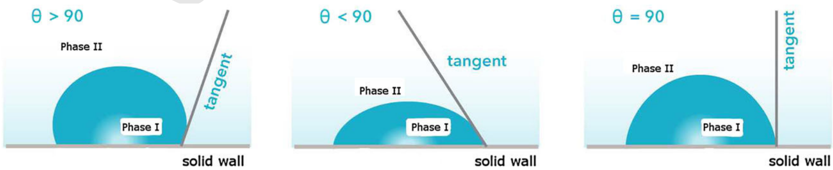

Fig. 1. Contact angle formed by the fluid–fluid interface with the solid boundary

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where $Q_{(s,t)} = \Omega \times (s, t)$, $0 \leqq s, t \leqq \infty$ and $Q_t = Q_{(0,t)}$. Let u_i be the volume fraction of fluid i $(i = 1, 2)$. We take the difference of volume fractions as an order parameter $\varphi := u_2 - u_1$. Then the values $\varphi = -1$ and $\varphi = 1$ represent the unmixed "pure" phases of fluid 1 and fluid 2, respectively. In terms of the order parameter φ, the volume averaged velocity of the binary mixture takes the following form:

$$\mathbf{v} = \frac{1-\varphi}{2}\mathbf{v}_1 + \frac{1+\varphi}{2}\mathbf{v}_2. \tag{1.2}$$

In addition, the mass difference depends linearly on the order parameter and the averaged density ρ of the mixture is given by

$$\rho(\varphi) = \frac{\rho_2 - \rho_1}{2}\varphi + \frac{\rho_1 + \rho_2}{2}, \tag{1.3}$$

where ρ_i is the specific densities of fluid i $(i = 1, 2)$. In system (1.1), $D\mathbf{v} = \frac{1}{2}(\nabla\mathbf{v} + \nabla\mathbf{v}^T)$ stands for the rate of deformation tensor, p denotes the fluid pressure, $\nu(\varphi) > 0$ is a viscosity coefficient and $m(\varphi) > 0$ is a (non-degenerate) mobility coefficient, both of them may depend on the order parameter φ. The relative mass flux $\mathbf{J}$ related to the diffusion of mixture components is given by

$$\mathbf{J} = -\rho'(\varphi)\, m(\varphi)\nabla\mu, \tag{1.4}$$

where $\mu = -\Delta\varphi + f(\varphi)$ is the chemical potential associated to φ. Moreover, $f = F'$ is the derivative of a homogeneous bulk potential density F for the binary mixture with a double-well structure. One of the physically relevant choices for F is the so-called logarithmic potential

$$F(s) = \frac{\Theta}{2}\big[(1+s)\log(1+s) + (1-s)\log(1-s)\big] - \frac{\Theta_0}{2}s^2, \quad s \in [-1, 1], \tag{1.5}$$

where $0 < \Theta < \Theta_0$ are positive constants denoting, respectively, the absolute temperature and the critical temperature of the mixture. Since a comparison principle for the fourth-order Cahn–Hilliard equation of φ is unknown, the singular behavior of f at ± 1 ensures that the order parameter φ takes values in the physically admissible interval $[-1, 1]$ along the evolution, while keeping the positivity of the averaged density $\rho(\varphi)$ in the general case of unmatched densities.

The diffuse interface model (1.1)–(1.5) was derived by Abels et al. [7] using methods from rational continuum mechanics. Here, we have taken the coefficient $a(\varphi, \nabla\varphi)$ in the chemical potential μ therein to be constant 1 for the sake of simplicity (cf. [7, (2.37)]). In the case of matched densities, that is, $\rho_1 = \rho_2$, the relative mass flux $\mathbf{J}$ simply vanishes and the system (1.1) reduces to the classical "model H" derived in [42] for the motion of an isothermal mixture of two immiscible and incompressible fluids subject to phase separation (cf. also [8,40,63,66]). On the other hand, for binary fluids with different densities, some other generalized diffuse interface models were proposed in the literature (see, for instance, [16,17,26,49]). The present model was derived using the volume averaged velocity (1.2), which entails a divergence free mean velocity field. Moreover, it has the nice features of being thermodynamically consistent and frame invariant (see [7, Remark 2.2]).

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There have been a considerable number of works devoted to the mathematical analysis of various diffuse interface models for two-phase flows. We refer to, for example, [1–3, 10, 14–16, 18, 31–33, 38, 40, 46, 75] and the references cited therein. Most of these papers deal with the following classical boundary and initial conditions:

$$\mathbf{v} = \mathbf{0}, \qquad \text{on } \Sigma_\infty, \tag{1.6}$$

$$\partial_{\mathbf{n}}\varphi = \partial_{\mathbf{n}}\mu = 0, \qquad \text{on } \Sigma_\infty, \tag{1.7}$$

$$\mathbf{v}|_{t=0} = \mathbf{v}_0, \ \ \varphi|_{t=0} = \varphi_0, \qquad \text{in } \Omega, \tag{1.8}$$

where $\Sigma_{(s,t)} = \Gamma \times (s, t)$ and $\Sigma_t = \Gamma_{(0,t)}$, with $\Gamma = \partial\Omega$ denoting the boundary of Ω and $\mathbf{n} = \mathbf{n}(x)$ being the exterior unit normal vector on Γ. System (1.1)–(1.5) (with a singular potential and a non-degenerate mobility), subject to (1.6)–(1.8), one was first analyzed in [5], where the authors established the existence of global weak solutions through a suitable implicit time discretization scheme. Their approach preserves the basic energy inequality at the discrete level and it allows one to avoid performing approximation of the singular potential F, which would be rather involved. Here we note that the singular potential forces the order parameter φ to take values only in $[-1, 1]$ and thus the linearly averaged density ρ (recall (1.3)) is bounded from above and below by some positive constants. The case of a regular potential (that is, defined on $\mathbb{R}$) and a degenerate mobility was then studied in [6], where existence of global weak solutions to system (1.1) subject to (1.6)–(1.8) was obtained. Moreover, the existence of global weak solutions to a non-Newtonian version of (1.1) with a regular potential F and a constant mobility was proven in [4]. Recently, a nonlocal variant of system (1.1) endowed with a no-slip boundary condition for the fluid velocity and a homogeneous Neumann boundary condition for the chemical potential as well as the initial condition (1.8) was considered in [29]. Assuming that the potential F is singular and the mobility is non-degenerate, the author of this work proved the existence of a global weak solution based on the Faedo-Galerkin method with the help of a three-level approximation of the original system.

We note that (1.6) yields a no-slip boundary condition for the fluid velocity, which is widely used in the literature on Navier–Stokes equations. In (1.7), the homogeneous Neumann boundary condition for the chemical potential μ entails that Γ is impenetrable and as a consequence, there is no mass flux of the components through the boundary. Together with (1.6), we can easily derive the mass conservation property, that is, the total mass $\int_\Omega \varphi(x, t)\mathrm{d}x$ is conserved for all $t \geqq 0$. Moreover, the condition $\partial_{\mathbf{n}}\varphi = 0$ on Γ describes a *static* contact angle of $\theta = \pi/2$ between the fluid–fluid free interface and the solid boundary of the domain at a contact line (cf. Fig. 1), which however turns out to be quite restrictive for many materials. Here, we are interested in the more physically relevant situation when one fluid may displace another immiscible fluid along the boundary Γ. This phenomenon effectively accounts for *moving contact lines* that result in a *dynamic* contact angle which deviates from the static one like $\pi/2$ above. In this case, the relative slipping between the fluids and the solid wall is in violation of the no-slip boundary conditions and thus new boundary conditions are required to describe the observed phenomena [27]. From detailed molecular dynamics studies, a generalization of the Navier boundary condition has been proposed in [57, 58] to account for

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the MCL problem. This generalized Navier boundary condition (GNBC in abbreviation) can be derived from the laws of thermodynamics and variational principles related to the minimum energy dissipation [55,56] (see also [61,62]). More precisely, denoting the interfacial free energy per unit area at the fluid-solid interface by $\widehat{G}(\varphi) = \frac{\zeta}{2}\varphi^2 + G(\varphi)$, where $\zeta > 0$ is a positive constant and $G(\varphi)$ is a certain nonlinear function, then for system (1.1)–(1.5) we replace (1.6)–(1.7) by the following no-flux boundary conditions

$$\mathbf{v} \cdot \mathbf{n} = 0, \quad \partial_{\mathbf{n}}\mu = 0, \quad \text{on } \Sigma_\infty, \tag{1.9}$$

together with a generalized Navier boundary condition for the velocity $\mathbf{v}$ and a dynamic boundary condition with surface convection for φ,

$$(2\nu(\varphi)\, D\mathbf{v} \cdot \mathbf{n})_{\boldsymbol{\tau}} + \beta(\varphi)\, \mathbf{v}_{\boldsymbol{\tau}} = \mathcal{L}(\varphi)\, \nabla_{\boldsymbol{\tau}}\varphi, \qquad \text{on } \Sigma_\infty, \tag{1.10}$$

$$\partial_t\varphi + \mathbf{v}_{\boldsymbol{\tau}} \cdot \nabla_{\boldsymbol{\tau}}\varphi = -l_0(\varphi)\, \mathcal{L}(\varphi), \qquad \text{on } \Sigma_\infty, \tag{1.11}$$

where

$$\mathcal{L}(\varphi) := -\Delta_{\boldsymbol{\tau}}\varphi + \partial_{\mathbf{n}}\varphi + \zeta\varphi + g(\varphi). \tag{1.12}$$

Here, $g = G'$, $\nabla_{\boldsymbol{\tau}}$ denotes the tangential gradient operator defined along the tangential direction $\boldsymbol{\tau} = (\tau_1, ..., \tau_{d-1})$ at Γ and $\Delta_{\boldsymbol{\tau}}$ denotes the Laplace-Beltrami operator on Γ. In general, for any vector $\mathbf{v} : \Gamma \to \mathbb{R}^d$, $\mathbf{v}_{\mathbf{n}} := (\mathbf{v}\cdot\mathbf{n})\mathbf{n}$ is the normal component of the vector field, while $\mathbf{v}_{\boldsymbol{\tau}} = \mathbf{v} - \mathbf{v}_{\mathbf{n}}$ corresponds to the tangential component of $\mathbf{v}$. Moreover, $l_0(\varphi) > 0$ is a certain relaxation coefficient, while $\beta(\varphi) > 0$ stands for a slip coefficient, both of them may locally depend on the composition φ. Related to the MCL problem, one typical choice of the energy density function $\widehat{G}$ takes the form $\widehat{G}(\varphi) = -\frac{\gamma}{2}\cos\theta_s \sin(\frac{\pi\varphi}{2})$, where θ_s is static contact angle and γ stands for the interfacial tension (see, for example, [54,58,59]). The generalized Navier boundary condition (1.10) indicates that the relative slipping is proportional to the sum of tangential viscous stress and the uncompensated Young stress $\mathcal{L}(\varphi)\nabla_{\boldsymbol{\tau}}\varphi$. On the other hand, the dynamic boundary condition (1.11) yields a relaxation dynamics of the order parameter φ that is linear in $\mathcal{L}(\varphi)$, that is, an Allen–Cahn type dynamics (with convection) for non-conserved quantities at the fluid-solid interface (see 4.2 for more details). We note that this choice is indeed not unique and a conserved dynamics of Cahn–Hilliard type for φ on the solid boundary may also be possible, see [48] for a recent attempt in this direction, where macroscopic effects of the flow is neglected for simplicity in the regime of slow dynamics.

The aim of this paper is to prove that the system (1.1)–(1.5) endowed with initial and boundary conditions (1.8)–(1.12) admits a global weak solution (see Theorem 2.2). To the best of our knowledge, only the special case of matched densities has been considered so far. This was done in [34], where the existence of a global energy solution was proven and, for a regular potential, the convergence of any such solution to a single equilibrium was also established. Several essential mathematical difficulties will be encountered due to the highly nonlinear structure of the PDE system and the complicated form of these non-classical boundary conditions. For instance, due to the current boundary conditions, it is not clear how to implement a suitable Galerkin type approximation since the test functions needed to derive the dissipative energy inequality will no longer be compatible with the possible

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truncations (see, for example, [34, Remark 3.1]). Next, the presence of the uncompensated Young stress $\mathcal{L}(\varphi)\nabla_{\boldsymbol{\tau}}\varphi$ and the boundary advection term $\mathbf{v}_{\boldsymbol{\tau}} \cdot \nabla_{\boldsymbol{\tau}}\varphi$ entail a strongly nonlinear boundary coupling for the system (1.1)–(1.5), which is rather difficult to handle. On the other hand, the combination of the dynamic boundary condition (1.11) with the singular potential F can produce additional strong singularities of the corresponding solutions close to the boundary (see [37,53], cf. also [23]). Moreover, as we shall see below, for the more general case with unmatched densities new difficulties related to the density function arise and the fixed-point argument used in [34] no longer seems applicable in a straight-forward way.

To resolve these mathematical issues, we shall combine and develop several techniques in recent works [4,5,29] concerning local, nonlocal or non-Newtonian versions of the diffuse interface system (1.1)–(1.5) that, nevertheless, are all related to standard boundary conditions like (1.6)–(1.7).

It is important to point out a basic feature of our problem, namely, the (formal) validity of the following dissipative energy law:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}E_{\text{tot}} &+ \int_\Omega 2\nu(\varphi)\,|D\mathbf{v}|^2\mathrm{d}x + \int_\Gamma \beta(\varphi)\,|\mathbf{v}_{\boldsymbol{\tau}}|^2\,\mathrm{d}S\\ &+ \int_\Omega m(\varphi)|\nabla\mu|^2\mathrm{d}x + \int_\Gamma l_0(\varphi)|\mathcal{L}(\varphi)\,|^2\mathrm{d}S = 0,\end{aligned} \tag{1.13}$$

where the total energy E_{tot} is given by the sum of the kinetic energy and the bulk/surface free energies:

$$\begin{aligned}E_{\text{tot}} := \frac{1}{2}\int_\Omega \rho\,(\varphi)\,|\mathbf{v}|^2\,\mathrm{d}x &+ \int_\Omega \left(\frac{1}{2}|\nabla\varphi|^2 + F(\varphi)\right)\mathrm{d}x\\ &+ \int_\Gamma \left(\frac{1}{2}|\nabla_{\boldsymbol{\tau}}\varphi|^2 + \frac{\zeta}{2}\,|\varphi|^2 + G(\varphi)\right)\mathrm{d}S.\end{aligned} \tag{1.14}$$

The energy identity (1.13) can be (formally) deduced by multiplying the first and third equations in (1.1) by $\mathbf{v}$, μ, respectively, integrating over Ω and testing (1.11) by $\mathcal{L}(\varphi)$ integrating over Γ, adding the resulting identies together and then applying integration by parts with the help of the incompressibility condition and the boundary conditions (1.9), (1.10). Identity (1.13) indeed serves as a starting point of our analysis though at the current stage we are only able to prove, even in two dimensions, that the weak solution satisfies an energy inequality.

Our strategy relies on a combination of suitable approximations and regularizations of the original system together with a novel time-implicit discretization scheme based on the energy dissipation law (1.13). First of all, we study a regularized problem by approximating the singular potential F with a family of regular potentials defined on $\mathbb{R}$. However, this regularization leads to the problem that the boundedness of φ can no longer be guaranteed and the averaged density ρ given by (1.3) may be meaningless outside the physical domain $[-1, 1]$ for φ (in particular, it may not be a priori bounded from below by a positive constant). This fact also causes difficulties for deriving the fundamental $L^\infty_t L^2_x$ -estimate of the velocity field $\mathbf{v}$ from the energy identity (1.13). To handle this issue, we shall extend the density function ρ in a nonlinear way from $[-1, 1]$ to the whole line $\mathbb{R}$ to preserve

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its boundedness properties (see (4.3)–(4.4) below). Following this approach, in order to preserve a dissipative energy identity in analogy with (1.13) that provides basic uniform estimates of the approximate solutions, we have to further modify the Navier–Stokes equations in (1.1) as follows (see also [4,29] for similar arguments):

$$\begin{aligned}&\partial_t(\rho\mathbf{v})+\operatorname{div}(\rho\mathbf{v}\otimes\mathbf{v})-\operatorname{div}(2\nu(\varphi)D\mathbf{v})+\nabla p+\operatorname{div}(\mathbf{v}\otimes\mathbf{J})\\&\quad=\mu\nabla\varphi+\frac{R}{2}\mathbf{v},\qquad\text{in } Q_\infty,\end{aligned}\tag{1.15}$$

where the extra term R is given by

$$R=-m(\varphi)\nabla\rho'(\varphi)\cdot\nabla\mu.\tag{1.16}$$

Then the above modified regularized problem can be solved as follows. First, in order to gain enough compactness to pass to the limit in this new "artificial" nonlinear term (1.16), we add a viscous term $\sigma\partial_t\varphi$ ($\sigma>0$) in the chemical potential μ and a non-Newtonian stress-like term $\varepsilon\left(\operatorname{div}(|D\mathbf{v}|^{q-2}D\mathbf{v})+|\mathbf{v}|^{q-2}\mathbf{v}\right)$ (for some $q>2d$ and $\varepsilon>0$) in the modified Navier–Stokes system (1.15). Then the resulting approximating problem can be solved through an implicit time discretization scheme in the spirit of [5]. Nonetheless, suitable modifications and extra efforts have to be made in order to handle those new boundary conditions (1.10)–(1.11). Next, for arbitrary but fixed positive parameters σ and ε, we proceed to solve the regularized problem with the original singular potential F by passing to the limit in the approximating family of regular potentials. This, in particular, implies that the limit function φ satisfies $\varphi\in[-1,1]$ and thus $R=0$ (see (1.16) and (4.3)), namely, the additional higher-order nonlinear term in (1.15) disappears. At this point, we will be able to recover the original momentum balance equation and collect all the necessary uniform bounds with respect to σ and ε. Finally, the existence of a global weak solution to the original problem will be obtained by passing to the limit as $\sigma\to0^+$ and $\varepsilon\to0^+$.

The plan of this paper goes as follows: in Section 2, we first summarize some notations and preliminary results. After that we introduce the necessary assumptions as well as the definition of weak solutions and then state our main result, that is, the existence of a global weak solution. In Section 3, we study a regularized system with regular approximating potentials and a nonlinear density function. The existence of weak solutions for this system is proven via an implicit time discretization scheme combined with the Leray–Schauder principle. In Section 4, after deriving necessary uniform estimates and then passing to the limit, we prove our main result. Finally, we provide a brief derivation of our diffuse interface model by variational principles in Appendix A and report some technical tools in Appendix B.

2. Existence of a Global Weak Solution

2.1. Preliminaries

We denote $a\otimes b=(a_ib_j)_{i,j=1}^d$ for vectors $a,b\in\mathbb{R}^d$ and $A_{\text{sym}}=\frac{1}{2}(A+A^T)$ for a matrix $A\in\mathbb{R}^{d\times d}$. If X is a (real) Banach space and X^* is its topological dual, then

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$\langle f, g\rangle \equiv \langle f, g\rangle_{X^*,X}$ for $f \in X^*$, $g \in X$, denotes the corresponding duality product. We write $X \overset{c}{\hookrightarrow} Y$ and $X \hookrightarrow Y$ if X is compactly (respectively, continuously) embedded into Y. The space $L^p(0, T; X)$ $(1 \leqq p \leqq \infty)$ denotes the set of all strongly measurable p -integrable functions or, if $p = \infty$, essentially bounded functions. Furthermore, the space $C([0, T]; X)$ denotes the Banach space of all bounded and continuous functions $u : [0, T] \to X$ equipped with the supremum norm and $C_w([0, T]; X)$ denotes the topological vector space of all bounded and weakly continuous functions $u : [0, T] \to X$. By $C_0^\infty(0, T; X)$ we denote the vector space of all smooth functions $u : (0, T) \to X$ with $\operatorname{supp}(u) \subset\subset (0, T)$. Finally, $u \in W^{1,p}(0, T; X)$, $1 \leqq p < \infty$, if and only if $u, \frac{\mathrm{d}u}{\mathrm{d}t} \in L^p(0, T; X)$, where $\frac{\mathrm{d}u}{\mathrm{d}t}$ denotes the vector-valued distributional derivative of u.

Let $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$ be a bounded domain with smooth boundary $\Gamma = \partial\Omega$. We denote by $L^p(\Omega)$, $L^p(\Gamma)$ $(1 \leqq p \leqq \infty)$ the usual Lebesgue spaces with norms $\|\cdot\|_{L^p}$ and $\|\cdot\|_{L^p(\Gamma)}$, respectively. Then for $s \geqq 0$ and $p \in [1, \infty)$, we denote by $H^{s,p}(\Omega)$ the Bessel-potential spaces and by $W^{s,p}(\Omega)$ the Slobodetskij spaces. One has $H^{s,2}(\Omega) = W^{s,2}(\Omega)$ for all s, but for $p \neq 2$ the identity $H^{s,p}(\Omega) = W^{s,p}(\Omega)$ is only true if $s \in \mathbb{N}_0$. If $s \in \mathbb{N}_0$, then $H^{s,p}(\Omega)$ and $W^{s,p}(\Omega)$ coincide with the usual Sobolev spaces. The corresponding function spaces over the boundary $\Gamma = \partial\Omega$ are defined via local charts. Let $\Upsilon_i : U_i \subset \mathbb{R}^{d-1} \to \Gamma$ be a finite family of parametrizations such that $\bigcup_i \Upsilon_i(U_i)$ covers Γ, and let $\{\psi_i\}$ be a partition of unity for Γ subordinate to this cover. Then for $s \geqq 0$ we have

$$H^{s,p}(\Gamma) = \left\{u \in L^p(\Gamma) : (\psi_i u) \circ \Upsilon_i \in H^{s,p}(\mathbb{R}^{d-1}) \text{ for all } i\right\},$$

with an equivalent norm given by $\|u\|_{H^{s,p}(\Gamma)} = \sum_i \|(\psi_i u) \circ \Upsilon_i\|_{H^{s,p}(\mathbb{R}^{d-1})}$. The spaces $W^{s,p}(\Gamma)$ are defined in the same manner, replacing H by W. In this way, the properties of the spaces over Ω described above easily carry over to the spaces over Γ. For $p \in (1, \infty)$ and $s > 1/p$ the trace of a function denoted by $\operatorname{tr}(u) = u|_\Gamma$ extends to a continuous operator

$$\operatorname{tr} : H^{s,p}(\Omega) \to W^{s-1/p,p}(\Gamma).$$

Here, we exclude the case $s - 1/p \in \mathbb{N}$ for $p \neq 2$. In the case $p = 2$ and $s \in \mathbb{N}_0$, we shall also use the standard notation $H^s := H^{s,2} = W^{s,2}$. In the Hilbert space setting, $(\cdot, \cdot)_{\mathcal{O}}$ stands for the usual scalar product which further induces the $L^2(\mathcal{O})$-norm, $\mathcal{O}$ being either a (measurable) subset of $\mathbb{R}^d$ or of $\mathbb{R}^d \times (0, T)$. Norms on $W^{s,p}(\Omega)$ and $W^{s,p}(\Gamma)$ will be indicated by $\|\cdot\|_{W^{s,p}}$ and $\|\cdot\|_{W^{s,p}(\Gamma)}$, respectively, for any $s \in \mathbb{R}$, $p \geqq 1$. Besides, we recall the following continuous embeddings: $H^1(\Gamma) \hookrightarrow L^\infty(\Gamma)$ if $d = 2$ and $H^1(\Gamma) \hookrightarrow L^q(\Gamma)$ for every $q \in [1, \infty)$ if $d = 3$; $H^{1/2}(\Gamma) \hookrightarrow L^s(\Gamma)$ for every $s \in [1, \infty)$ if $d = 2$ and for $s = 4$ if $d = 3$.

Following the notation used in [34], we define the spaces

$$V^s = \left\{(\varphi, \psi) \in H^s(\Omega) \times H^{s-1/2}(\Gamma) : \psi = \operatorname{tr}(\varphi) \in H^s(\Gamma)\right\}, \quad s \in \mathbb{N},$$

equipped with norms given by

$$\|(\varphi, \psi)\|_{V^s}^2 = \|\varphi\|_{H^s}^2 + \|\psi\|_{H^s(\Gamma)}^2 .$$

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In particular, we shall set

$$\|(\varphi,\psi)\|_{V^1}^2 := \int_\Omega |\nabla\varphi|^2\,\mathrm{d}x + \int_\Gamma \left(|\nabla_{\boldsymbol{\tau}}\psi|^2 + \zeta\,|\psi|^2\right)\mathrm{d}S$$

for some $\zeta > 0$. Note that $V^s \overset{c}{\hookrightarrow} V^{s-1}$ for $s \in \mathbb{N}$.

We now introduce the functional framework associated with the velocity field. To this end, we consider a (real) Hilbert space X and denote by $\mathbb{X}$ the vector space $X \times \cdots \times X$ (d-times), endowed with the product structure, and by $\mathbb{X}^*$ its dual; $\|\cdot\|_{\mathbb{X}^*}$ will denote the dual norm of $\|\cdot\|_{\mathbb{X}}$ on $\mathbb{X}^*$. Then we introduce (with some abuse of notation) the spaces $\mathbb{H} := \mathbb{H}^0$ and $\mathbb{H}^s$ ($s > 0$), defined by

$$\mathbb{H} := \overline{\mathbb{C}^\infty_{\mathrm{div}}\left(\overline{\Omega}\right)}^{\mathbb{L}^2(\Omega)} \quad\text{and}\quad \mathbb{H}^s := \overline{\mathbb{C}^\infty_{\mathrm{div}}\left(\overline{\Omega}\right)}^{\mathbb{W}^{s,2}(\Omega)}, \tag{2.1}$$

where

$$\mathbb{C}^\infty_{\mathrm{div}}\left(\overline{\Omega}\right) = \left\{\mathbf{u} \in \mathbb{C}^\infty\left(\overline{\Omega}\right) : \nabla\cdot\mathbf{u} = 0 \text{ in } \Omega,\ \mathbf{u}\cdot\mathbf{n} = 0 \text{ on } \Gamma\right\}.$$

The corresponding Helmholtz–Leray projection is denoted by $\mathbb{P}$, such that $\mathbb{P}f = f - \nabla p$, where $p \in H^1(\Omega)$, $\int_\Omega p\mathrm{d}x = 0$, is the solution of the weak Neumann problem

$$(\nabla p, \nabla\varphi)_\Omega = (f, \nabla\varphi)_\Omega, \quad \forall\varphi \in C^\infty(\overline{\Omega}). \tag{2.2}$$

2.2. Statement of the Main Result

First, we introduce some necessary assumptions to formulate the notion of a weak solution to our problem.

Assumption 1. We assume that $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, is a bounded domain with a smooth boundary of class $\mathcal{C}^2$. In addition, we impose the following conditions:

(1) The density function ρ is given by

$$\rho(r) = \frac{\rho_2 - \rho_1}{2} r + \frac{\rho_1 + \rho_2}{2}, \quad \forall r \in [-1, 1],$$

where the constants $\rho_1, \rho_2 > 0$ are specific densities of the corresponding two fluids.

(2) We assume that $m, l_0 \in C^{1,1}_{\mathrm{loc}}(\mathbb{R})$, $\nu, \beta \in C^{0,1}_{\mathrm{loc}}(\mathbb{R})$ and

$$0 < m_0 \leqq l_0(s),\ m(s),\ \nu(s),\ \beta(s) \leqq M_0$$

for some given constants $m_0, M_0 > 0$.

(3) The free energy densities are given by

$$F(r) = F_0(r) - \frac{c_F}{2} r^2 \ \text{ for some } c_F \in \mathbb{R}, \quad \text{and } G(r) = \int_0^r g(\xi)\,\mathrm{d}\xi,$$

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satisfying $F_0 \in C([-1,1]) \cap C^2(-1,1)$ with $F_0(0) = 0$ and $G \in C^2(\mathbb{R})$. For $f_0 = F_0' \in C^1(-1,1)$, we assume that $f_0(0) = 0$, $f_0'(r) \geqq 0$ for $r \in (-1,1)$ and

$$\lim_{r \to \pm 1} f_0(r) = \pm\infty, \qquad \lim_{r \to \pm 1} f_0'(r) = +\infty.$$

Besides, there exist constants $C_g > 0$ and $c_G \geqq 0$ such that

$$|g'(r)| \leqq C_g(1+|r|^p), \quad g'(r) \geqq -c_G, \quad G(r) \geqq -c_G, \tag{2.3}$$

where $p \in [1,\infty)$ is fixed, but arbitrary for $d = 2, 3$.

(4) There exist constants $M \in (0,1)$, $\delta > 0$, $C_{\delta,M} > 0$ and $C_M > 0$ such that

$$f_0'(s) - \delta(f_0(s))^2 \geqq -C_{\delta,M}, \qquad \text{for any } s \in (-1,-M] \cup [M,1), \tag{2.4}$$

$$f_0(s)\widehat{g}(s) \geqq -C_M, \qquad \text{for any } s \in (-1,-M] \cup [M,1), \tag{2.5}$$

where $\widehat{g}(s) = g(s) + \zeta s$.

Remark 2.1. Assumptions (2.4) and (2.5) can be regarded as certain technical assumptions for the existence of global weak solutions (cf., for example, [34]). Nevertheless, they are fulfilled by a wide range of nonlinearities satisfying the condition (3) above. For instance, (2.4) is satisfied by the classical logarithmic function

$$f_0(s) = c_0 \ln\left(\frac{1+s}{1-s}\right), \quad \text{for some } c_0 > 0.$$

Moreover, condition (2.5) can be satisfied by the above f_0 as long as $\pm\widehat{g}(\pm 1) > 0$, that is, the function $\widehat{g}(s) = g(s) + \zeta s$ shares the same sign as the singular potential f_0 near its singular points ± 1. The later sign condition on $\widehat{g}$ turns out to be natural in the study of the Cahn–Hilliard equation with dynamic boundary conditions and singular potentials (see [37,53]). Indeed, this sign condition can be further relaxed in view of (2.5). In particular, we recall that the typical interfacial free energy density at the fluid-solid interface for the moving contact line problem is $\widehat{G}(s) = -\frac{\gamma}{2}\cos\theta_s \sin(\frac{\pi s}{2})$ (see, for example, [58,59]). Then we have

$$\widehat{g}(s) = -\frac{\gamma\pi}{4}\cos\theta_s \cos\left(\frac{\pi s}{2}\right),$$

and it is easy to verify that assumption (2.5) is fulfilled for this choice of $\widehat{g}$ together with the logarithmic potential f_0, since $\lim_{s\to\pm 1} f_0(s)\widehat{g}(s) = 0$.

Inspired by [52], it will be convenient to view the trace of the order parameter φ as an unknown variable on the boundary Γ. Thus, in the following text, we shall use the new variable

$$\psi := \mathrm{tr}(\varphi).$$

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Then the original problem (1.1)–(1.5) subject to the initial and boundary conditions (1.8)–(1.12) can be rewritten into the following form:

$$\begin{cases} \partial_t(\rho\mathbf{v}) + \operatorname{div}(\rho\mathbf{v}\otimes\mathbf{v}) - \operatorname{div}(2\nu(\varphi)D\mathbf{v}) + \nabla p \\ \qquad + \operatorname{div}(\mathbf{v}\otimes\mathbf{J}) = \mu\nabla\varphi, & \text{in } Q_\infty, \\ \operatorname{div}\mathbf{v} = 0, & \text{in } Q_\infty, \\ \partial_t\varphi + \mathbf{v}\cdot\nabla\varphi = \operatorname{div}\left(m(\varphi)\nabla\mu\right), & \text{in } Q_\infty, \\ \mu = -\Delta\varphi + f(\varphi), & \text{in } Q_\infty, \\ \rho(\varphi) = \dfrac{\rho_2-\rho_1}{2}\varphi + \dfrac{\rho_1+\rho_2}{2}, & \text{in } Q_\infty, \\ \mathbf{J} = -\rho'(\varphi)\, m(\varphi)\nabla\mu, & \text{in } Q_\infty, \end{cases} \tag{2.6}$$

subject to the boundary conditions

$$\mathbf{v}\cdot\mathbf{n} = 0, \qquad \text{on } \Sigma_\infty, \tag{2.7}$$

$$(2\nu(\varphi)\, D\mathbf{v}\cdot\mathbf{n})_{\boldsymbol{\tau}} + \beta(\psi)\,\mathbf{v}_{\boldsymbol{\tau}} = \mathcal{L}(\psi)\,\nabla_{\boldsymbol{\tau}}\psi, \qquad \text{on } \Sigma_\infty, \tag{2.8}$$

$$\varphi = \psi, \quad \partial_{\mathbf{n}}\mu = 0, \qquad \text{on } \Sigma_\infty, \tag{2.9}$$

$$\partial_t\psi + \mathbf{v}_{\boldsymbol{\tau}}\cdot\nabla_{\boldsymbol{\tau}}\psi = -l_0(\psi)\,\mathcal{L}(\psi), \qquad \text{on } \Sigma_\infty, \tag{2.10}$$

with

$$\mathcal{L}(\psi) := -\Delta_{\boldsymbol{\tau}}\psi + \partial_{\mathbf{n}}\varphi + \zeta\psi + g(\psi), \qquad \text{on } \Sigma_\infty, \tag{2.11}$$

as well as to the initial conditions

$$\mathbf{v}|_{t=0} = \mathbf{v}_0, \quad \varphi|_{t=0} = \varphi_0, \quad \psi|_{t=0} = \psi_0 = \operatorname{tr}(\varphi_0), \quad \text{in } \Omega. \tag{2.12}$$

Remark 2.2. (1) If the solution $(\mathbf{v}, \varphi)$ to the original problem (1.1)–(1.5) subject to (1.8)–(1.12) is sufficiently regular (for instance, φ is regular enough that its trace makes sense), then the above two systems are equivalent. Conversely, the conclusion is also true.

(2) From the mathematical point of view, the evolution equation (1.11) serves as a (nontrivial) boundary condition that is necessary for the solvability of the fourth-order Cahn–Hilliard equation in a bounded domain Ω (another one is $\partial_{\mathbf{n}}\mu = 0$), see for example, [19,37,52,53,72]. We recall that in the classical setting of the Cahn–Hilliard equation, this condition (1.11) is replaced by the simpler one $\partial_{\mathbf{n}}\varphi = 0$ (see, for example, [1,31,38,75] and references therein). On the other hand, the nontrivial bulk-boundary interaction is more clearly described in the above reformulation (2.6)–(2.12). Indeed, the bulk order parameter φ can be viewed as a solution to the Cahn–Hilliard equation in Ω endowed with a nonhomogeneous Dirichlet boundary condition $\varphi = \psi$ and a homogeneous boundary condition $\partial_{\mathbf{n}}\mu = 0$ on $\partial\Omega$, where the boundary datum ψ is now determined by an Allen–Cahn type evolution equation (2.10) on $\partial\Omega$.

Here we introduce the notion of weak solutions.

Definition 2.1. Let $T \in (0, \infty)$ be an arbitrary but fixed constant. Suppose that Assumption 1 is satisfied, $\mathbf{v}_0 \in \mathbb{H}$, $(\varphi_0, \psi_0) \in V^1$, $F_0(\varphi_0) \in L^1(\Omega)$, $F_0(\psi_0) \in$

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$L^1(\Gamma)$ and $\frac{1}{|\Omega|}\int_\Omega \varphi_0 \mathrm{d}x \in (-1,1)$. A quadruplet $(\mathbf{v}, \mu, \varphi, \psi)$ with the following properties:

$$\mathbf{v} \in C_w([0,T];\mathbb{H}) \cap L^2(0,T;\mathbb{H}^1),$$
$$(\varphi, \psi) \in C_w([0,T];V^1) \cap L^2(0,T;V^2),$$
$$\mu \in L^2(0,T;H^1(\Omega)), \quad \mathcal{L}(\psi) \in L^2(0,T;L^2(\Gamma)),$$

is a weak solution to problem (2.6)–(2.12) (or, problem (1.1)–(1.5) subject to (1.8)–(1.12)) on $[0,T]$, if the following conditions are satisfied:

$$\begin{aligned} &-(\rho\mathbf{v}, \partial_t \mathbf{w})_{Q_T} + (\mathrm{div}(\rho\mathbf{v}\otimes\mathbf{v}), \mathbf{w})_{Q_T} + (2\nu(\varphi)D\mathbf{v}, D\mathbf{w})_{Q_T} + (\beta(\psi)\mathbf{v}_{\boldsymbol{\tau}}, \mathbf{w}_{\boldsymbol{\tau}})_{\Sigma_T} \\ &\quad = ((\mathbf{v}\otimes\mathbf{J}), \nabla\mathbf{w})_{Q_T} + (\mu\nabla\varphi, \mathbf{w})_{Q_T} + (\mathcal{L}(\psi)\nabla_{\boldsymbol{\tau}}\psi, \mathbf{w}_{\boldsymbol{\tau}})_{\Sigma_T}, \end{aligned} \tag{2.13}$$

for all $\mathbf{w} \in C_0^\infty(0,T;\mathbb{C}^\infty_{\mathrm{div}}(\overline{\Omega}))$,

$$-(\varphi, \partial_t\xi)_{Q_T} + (\mathbf{v}\cdot\nabla\varphi, \xi)_{Q_T} = -(m(\varphi)\nabla\mu, \nabla\xi)_{Q_T}, \tag{2.14}$$
$$-(\psi, \partial_t\theta)_{\Sigma_T} + (\mathbf{v}_{\boldsymbol{\tau}}\cdot\nabla_{\boldsymbol{\tau}}\psi, \theta)_{\Sigma_T} = -(l_0(\psi)\mathcal{L}(\psi), \theta)_{\Sigma_T}, \tag{2.15}$$

for all $\xi \in C_0^\infty(0,T;C^1(\overline{\Omega}))$, $\theta \in C_0^\infty(0,T;C(\Gamma))$,

$$\mu = -\Delta\varphi + f(\varphi), \qquad \text{almost everywhere in } Q_T, \tag{2.16}$$
$$\mathcal{L}(\psi) = -\Delta_{\boldsymbol{\tau}}\psi + \partial_{\mathbf{n}}\varphi + \zeta\psi + g(\psi), \qquad \text{almost everywhere in } \Sigma_T, \tag{2.17}$$
$$\rho(\varphi) = \frac{\rho_2-\rho_1}{2}\varphi + \frac{\rho_1+\rho_2}{2}, \qquad \text{almost everywhere in } Q_T, \tag{2.18}$$
$$\mathbf{J} = \frac{\rho_1-\rho_2}{2}m(\varphi)\nabla\mu, \qquad \text{almost everywhere in } Q_T, \tag{2.19}$$
$$|\varphi| < 1, \qquad \text{almost everywhere in } Q_T, \tag{2.20}$$
$$|\psi| \leqq 1, \qquad \text{almost everywhere in } \Sigma_T, \tag{2.21}$$

and $(\mathbf{v}, \varphi, \psi)|_{t=0} = (\mathbf{v}_0, \varphi_0, \psi_0)$. Moreover, the energy inequality

$$\begin{aligned} &E_{\mathrm{tot}}(\mathbf{v}(t), \varphi(t), \psi(t)) + \int_{Q_{(s,t)}} 2\nu(\varphi)|D\mathbf{v}|^2 \mathrm{d}x\mathrm{d}\tau + \int_{\Sigma_{(s,t)}} \beta(\psi)|\mathbf{v}_{\boldsymbol{\tau}}|^2 \mathrm{d}S\mathrm{d}\tau \\ &\quad + \int_{Q_{(s,t)}} m(\varphi)|\nabla\mu|^2 \mathrm{d}x\mathrm{d}\tau + \int_{\Sigma_{(s,t)}} l_0(\psi)|\mathcal{L}(\psi)|^2 \mathrm{d}S\mathrm{d}\tau \\ &\quad \leqq E_{\mathrm{tot}}(\mathbf{v}(s), \varphi(s), \psi(s)) \end{aligned} \tag{2.22}$$

holds for all $t \in [s,\infty)$ and almost all $s \in [0,\infty)$ (including $s = 0$), where the total energy E_{tot} is given by

$$\begin{aligned} E_{\mathrm{tot}}(\mathbf{v}, \varphi, \psi) := &\frac{1}{2}\int_\Omega \rho(\varphi)|\mathbf{v}|^2 \mathrm{d}x + \int_\Omega \left(\frac{1}{2}|\nabla\varphi|^2 + F(\varphi)\right)\mathrm{d}x \\ &+ \int_\Gamma \left(\frac{1}{2}|\nabla_{\boldsymbol{\tau}}\psi|^2 + \frac{\zeta}{2}|\psi|^2 + G(\psi)\right)\mathrm{d}S. \end{aligned} \tag{2.23}$$

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Remark 2.3. The assumption $\frac{1}{|\Omega|}\int_\Omega \varphi_0 \mathrm{d}x \in (-1, 1)$ indicates that the initial datum is not allowed to be a pure state (that is, ± 1). On the other hand, if the initial datum is a pure state, then no separation process will take place, because we now have a single fluid whose dynamics can be modeled by the Navier–Stokes equations (and some other variants, see for instance, [35] and the references therein).

We are now in a position to state the main result of the paper.

Theorem 2.2. (Existence of a global weak solution) *Let Assumption 1 hold. Suppose that* $\mathbf{v}_0 \in \mathbb{H}$, $(\varphi_0, \psi_0) \in V^1$ *with* $F_0(\varphi_0) \in L^1(\Omega)$, $F_0(\psi_0) \in L^1(\Gamma)$ *and* $\frac{1}{|\Omega|}\int_\Omega \varphi_0 dx \in (-1, 1)$. *Then for any* $T \in (0, \infty)$, *there exists a global weak solution* $(\mathbf{v}, \mu, \varphi, \psi)$ *to problem* (1.1)–(1.5) *subject to* (1.8)–(1.12) *on* $[0, T]$ *in the sense of Definition 2.1.*

Remark 2.4. Due to the highly nonlinear structure of our system (both in the bulk and on the boundary) and the presence of the singular bulk potential, uniqueness of weak solutions in the two dimensional case is still an open issue (even in the case of matched densities, see [34]).

Remark 2.5. Comparing with [59], in our system we include an additional Laplace-Beltrami operator in the boundary condition (see (1.12)). On one hand, the term $\Delta_\tau \psi$ corresponds to possible surface diffusion effect on the boundary Γ. This appears physically meaningful since it also seems to have a damping effect on the dynamics near Γ (cf. [30]). On the other hand, it is crucial from the mathematical point of view since this term provides extra regularity for the boundary order parameter ψ (see Lemma B.4 and, for further discussion, see [30]). In particular, it plays an important role in obtaining sufficient strong uniform estimates to pass to the limit (see also [34, Remark 3.4]). Without this surface diffusion term in (1.12), whether the problem (1.1)–(1.5) subject to (1.8)–(1.12) admits a global weak solution remains an open problem even in the case of matched densities (cf. [34]). For attempts to study the fluid-free case without surface diffusion and its variants we refer, for instance, to [19,30,37,48,71].

3. An Approximating Problem with Regular Bulk Potential

The proof of Theorem 2.2 will be carried out through several steps (cf. Introduction). First, we shall consider the following two-parameter approximating system with a regular bulk potential:

$$
\begin{cases}
\partial_t(\rho\mathbf{v}) + \mathrm{div}(\rho\mathbf{v}\otimes\mathbf{v}) - \mathrm{div}(2\nu(\varphi)D\mathbf{v}) + \nabla p + \mathrm{div}(\mathbf{v}\otimes\mathbf{J}) & \\
\quad + \varepsilon\Big(\mathrm{div}(|D\mathbf{v}|^{q-2}D\mathbf{v}) + |\mathbf{v}|^{q-2}\mathbf{v}\Big) = \mu\nabla\varphi + \dfrac{R}{2}\mathbf{v}, & \text{in } Q_\infty,\\
\mathrm{div}\,\mathbf{v} = 0, & \text{in } Q_\infty,\\
\partial_t\varphi + \mathbf{v}\cdot\nabla\varphi = \mathrm{div}\,(m(\varphi)\nabla\mu), & \text{in } Q_\infty,\\
\mu = -\Delta\varphi + f(\varphi) + \sigma\partial_t\varphi, & \text{in } Q_\infty,\\
\mathbf{J} = -\rho'(\varphi)\,m(\varphi)\nabla\mu, & \text{in } Q_\infty,\\
R = -m(\varphi)\,\nabla\rho'(\varphi)\cdot\nabla\mu, & \text{in } Q_\infty,
\end{cases}
\tag{3.1}
$$

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for some $\sigma, \varepsilon \in [0,1]$ and $q > 2d$. The regularized system (3.1) is equipped with the initial and boundary conditions (1.8)–(1.11), with the exception of (1.10) which now reads

$$\varepsilon(|D\mathbf{v}|^{q-2}\, D\mathbf{v}\cdot\mathbf{n})_{\boldsymbol{\tau}} + (2\nu(\varphi)\, D\mathbf{v}\cdot\mathbf{n})_{\boldsymbol{\tau}} + \beta(\psi)\,\mathbf{v}_{\boldsymbol{\tau}} = \mathcal{L}(\psi)\,\nabla_{\boldsymbol{\tau}}\psi, \quad \text{on } \Sigma_\infty.$$

In the text that follows, the resulting initial boundary value problem of system (3.1) will be referred to as $(S_{\sigma,\varepsilon})$.

Now we state our assumptions in order to solve problem $(S_{\sigma,\varepsilon})$.

Assumption 2. We assume that $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$ is a bounded domain with a smooth boundary of class $\mathcal{C}^2$ and additionally we impose the following conditions:

(1) Instead of the linear form (1.3), the density function satisfies $\rho \in C^2(\mathbb{R})$, $\rho \geqq \rho_0$ for some constant $\rho_0 > 0$, and ρ, ρ', ρ'' are bounded in $\mathbb{R}$.
(2) $m, l_0 \in C^{1,1}_{\mathrm{loc}}(\mathbb{R})$, $\nu, \beta \in C^{0,1}_{\mathrm{loc}}(\mathbb{R})$ such that $0 < m_0 \leqq l_0(s), m(s), \nu(s), \beta(s) \leqq M_0$ for some given constants $m_0, M_0 > 0$.
(3) The free energy densities given by

$$F(r) = \int_0^r f(\zeta)\mathrm{d}\zeta \in C^2(\mathbb{R}), \quad G(r) = \int_0^r g(\zeta)\mathrm{d}\zeta \in C^2(\mathbb{R})$$

satisfy the following assumptions: there exist $c_F, c_G \geqq 0$ and $C_f, C_g > 0$ such that

$$\left|f'(r)\right| \leqq C_f\left(1+|r|^p\right), \quad f'(r) \geqq -c_F, \quad F(r) \geqq -c_F, \tag{3.2}$$
$$\left|g'(r)\right| \leqq C_g(1+|r|^q), \quad g'(r) \geqq -c_G, \quad G(r) \geqq -c_G, \tag{3.3}$$

for any $r \in \mathbb{R}$. Here, $p, q \in [1,\infty)$ are arbitrary if $d = 2$, and $p = 2$, $q \in [1,\infty)$ being arbitrary if $d = 3$.

Remark 3.1. In (3.1) we include a non-Newtonian type regularizing term in the modified Navier–Stokes system (cf. [4]) and also a standard viscous term in the chemical potential μ. The regularization of the original system (1.1)–(1.5) through these additional terms allows us to handle successfully the extra term R, whose presence is due to the nonlinear extension of the averaged density ρ (cf. (1) of Assumption 2 and see Introduction).

Next, we introduce the notion of weak solution for problem $(S_{\sigma,\varepsilon})$.

Definition 3.1. Let $T \in (0,\infty)$ be given, but otherwise arbitrary. Let $\mathbf{v}_0 \in \mathbb{H}$, $(\varphi_0, \psi_0) \in V^1$ and Assumption 2 be satisfied. A quadruplet $(\mathbf{v}, \mu, \varphi, \psi)$ with the properties

$$\mathbf{v} \in C_w([0,T];\mathbb{H}) \cap L^2(0,T;\mathbb{H}^1),$$
$$(\varphi, \psi) \in C_w([0,T];V^1) \cap L^2(0,T;V^2),$$
$$\mu \in L^2(0,T;H^1(\Omega)), \quad \mathcal{L}(\psi) \in L^2(0,T;L^2(\Gamma)),$$

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is a weak solution to the approximating problem $(S_{\sigma,\varepsilon})$ if the following conditions are satisfied:

$$\begin{aligned}
&-(\rho\mathbf{v},\partial_t\mathbf{w})_{Q_T}+(\operatorname{div}(\rho\mathbf{v}\otimes\mathbf{v}),\mathbf{w})_{Q_T}+(2\nu(\varphi)D\mathbf{v},D\mathbf{w})_{Q_T}\\
&\quad+(\beta(\psi)\mathbf{v}_{\boldsymbol{\tau}},\mathbf{w}_{\boldsymbol{\tau}})_{\Sigma_T}+\varepsilon\left(|D\mathbf{v}|^{q-2}D\mathbf{v},D\mathbf{w}\right)_{Q_T}+\varepsilon\left(|\mathbf{v}|^{q-2}\mathbf{v},\mathbf{w}\right)_{Q_T}\\
&=((\mathbf{v}\otimes\mathbf{J}),\nabla\mathbf{w})_{Q_T}+\frac{1}{2}(R\mathbf{v},\mathbf{w})_{Q_T}+(\mu\nabla\varphi,\mathbf{w})_{Q_T}\\
&\quad+(\mathcal{L}(\psi)\nabla_{\boldsymbol{\tau}}\psi,\mathbf{w}_{\boldsymbol{\tau}})_{\Sigma_T}, \qquad (3.4)
\end{aligned}$$

for all $\mathbf{w}\in C_0^\infty(0,T;\mathbb{C}^\infty_{\operatorname{div}}(\overline{\Omega}))$,

$$-(\varphi,\partial_t\xi)_{Q_T}+(\mathbf{v}\cdot\nabla\varphi,\xi)_{Q_T}=-(m(\varphi)\nabla\mu,\nabla\xi)_{Q_T}, \qquad (3.5)$$

$$-(\psi,\partial_t\theta)_{\Sigma_T}+(\mathbf{v}_{\boldsymbol{\tau}}\cdot\nabla_{\boldsymbol{\tau}}\psi,\theta)_{\Sigma_T}=-(l_0(\psi)\mathcal{L}(\psi),\theta)_{\Sigma_T}, \qquad (3.6)$$

for all $\xi\in C_0^\infty(0,T;C^1(\overline{\Omega}))$, $\theta\in C_0^\infty(0,T;C(\Gamma))$,

$$\mu=-\Delta\varphi+f(\varphi)+\sigma\partial_t\varphi, \qquad \text{almost everywhere in } Q_T, \qquad (3.7)$$

$$\mathcal{L}(\psi)=-\Delta_{\boldsymbol{\tau}}\psi+\partial_{\mathbf{n}}\varphi+\zeta\psi+g(\psi), \qquad \text{almost everywhere in } \Sigma_T, \qquad (3.8)$$

and $(\mathbf{v},\varphi,\psi)|_{t=0}=(\mathbf{v}_0,\varphi_0,\psi_0)$. The flux $\mathbf{J}$ satisfies (1.4) almost everywhere in Q_T and

$$(R\mathbf{v},\mathbf{w})_{Q_T}=-\int_{Q_T}m(\varphi)\left(\nabla\rho'(\varphi)\cdot\nabla\mu\right)\mathbf{v}\cdot\mathbf{w}\,\mathrm{d}x\,\mathrm{d}t, \qquad (3.9)$$

for all $\mathbf{w}\in C_0^\infty(0,T;\mathbb{C}^\infty_{\operatorname{div}}(\overline{\Omega}))$.

Remark 3.2. We note that according to the definitions of $\mathbf{J}$ and R (recall (1.4) and (1.16)), the third equation of (3.1) for φ indeed implies that

$$\partial_t\rho+\operatorname{div}(\rho\mathbf{v}+\mathbf{J})=R, \quad \text{in } Q_T. \qquad (3.10)$$

In this case, a weak formulation of (3.10) reads

$$-(\rho(\varphi),\partial_t\varpi)_{Q_T}+(\operatorname{div}(\rho\mathbf{v}+\mathbf{J}),\varpi)_{Q_T}=(R,\varpi)_{Q_T}$$

for all $\varpi\in C_0^\infty(0,T;C^1(\overline{\Omega}))$.

The main result of this section is the following existence theorem for the approximating problem $(S_{\sigma,\varepsilon})$:

Theorem 3.2. *Let Assumption 2 be satisfied. Suppose that $\sigma,\varepsilon\in(0,1]$, $\mathbf{v}_0\in\mathbb{H}$ and $(\varphi_0,\psi_0)\in V^1$. Then for any $T>0$, there exists a global weak solution $(\mathbf{v},\mu,\varphi,\psi)$ of the approximating problem $(S_{\sigma,\varepsilon})$ in the sense of Definition 3.1. In addition, we have*

$$\sigma^{1/2}\partial_t\varphi\in L^2\left(0,T;L^2(\Omega)\right), \quad \varepsilon^{1/q}\mathbf{v}\in L^q\left(0,T;W^{1,q}(\Omega)\right).$$

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Also, every weak solution satisfies the following (modified) energy inequality:

$$
\begin{aligned}
&E_{\mathrm{tot}}(\mathbf{v}(t), \varphi(t), \psi(t)) + \int_{Q_{(s,t)}} 2\nu(\varphi)\,|D\mathbf{v}|^2 dx d\tau + \int_{\Sigma_{(s,t)}} \beta(\psi)\,|\mathbf{v}_{\boldsymbol{\tau}}|^2\, dS d\tau \\
&\quad + \int_{Q_{(s,t)}} m(\varphi)|\nabla\mu|^2 dx d\tau + \int_{\Sigma_{(s,t)}} l_0(\psi)|\mathcal{L}(\psi)|^2 dS d\tau \\
&\quad + \sigma \int_{Q_{(s,t)}} |\partial_t\varphi|^2\, dx d\tau + \varepsilon \int_{Q_{(s,t)}} \left(|D\mathbf{v}|^q + |\mathbf{v}|^q\right) dx d\tau \\
&\quad \leq E_{\mathrm{tot}}(\mathbf{v}(s), \varphi(s), \psi(s)),
\end{aligned}
\tag{3.11}
$$

for all $t \in [s, \infty)$ and almost all $s \in [0, \infty)$ (including $s = 0$), where the total energy E_{tot} is given by (2.23) *with F and G satisfying* (3) *of Assumption 2.*

Theorem 3.2 will be proven by means of a suitable implicit time discretization scheme in the spirit of [5], combined with a delicate compactness argument.

3.1. An Implicit Time Discretization Scheme

To set up our implicit time discretization, we consider the time step $h = \frac{1}{N}$ for $N \in \mathbb{N}_0$ and the elements $\mathbf{v}_k \in \mathbb{H}$, $(\varphi_k, \psi_k) \in V^1$ with $f(\varphi_k) \in L^2(\Omega)$, $g(\psi_k) \in L^2(\Gamma)$ and $\rho_k = \rho(\varphi_k)$ be given. Then we construct

$$
(\mathbf{v}, \mu, \varphi, \psi) = (\mathbf{v}_{k+1}, \mu_{k+1}, \varphi_{k+1}, \psi_{k+1})
$$

as a solution, with

$$
\mathbf{J} = \mathbf{J}_{k+1} := -\rho'(\varphi_k)\, m(\varphi_k) \nabla \mu_{k+1} = -\rho'(\varphi_k)\, m(\varphi_k) \nabla \mu, \tag{3.12}
$$

to the following nonlinear system: find $(\mathbf{v}, \mu, \varphi, \psi)$ with $\mathbf{v} \in \mathbb{H}^1$, $(\varphi, \psi) \in V^2$ and $\mu \in H^2_n(\Omega) = \{u \in H^2(\Omega) : \partial_{\mathbf{n}} u = 0 \text{ on } \Gamma\}$, such that

$$
\begin{aligned}
&\left(\frac{\rho\mathbf{v} - \rho_k\mathbf{v}_k}{h}, \mathbf{w}\right)_\Omega + (\mathrm{div}(\rho_k\mathbf{v}\otimes\mathbf{v}), \mathbf{w})_\Omega + (2\nu(\varphi_k) D\mathbf{v}, D\mathbf{w})_\Omega \\
&\qquad + (\beta(\psi_k)\mathbf{v}_{\boldsymbol{\tau}}, \mathbf{w}_{\boldsymbol{\tau}})_\Gamma + \varepsilon\left(|D\mathbf{v}|^{q-2} D\mathbf{v}, D\mathbf{w}\right)_\Omega + \varepsilon\left(|\mathbf{v}|^{q-2}\mathbf{v}, \mathbf{w}\right)_\Omega \\
&\quad = (\mu\nabla\varphi_k, \mathbf{w})_\Omega - (\mathrm{div}(\mathbf{v}\otimes\mathbf{J}), \mathbf{w})_\Omega \\
&\qquad + \frac{1}{2}\left(\left(\frac{\rho - \rho_k}{h} + \mathrm{div}\,(\rho_k\mathbf{v} + \mathbf{J})\right)\mathbf{v}, \mathbf{w}\right)_\Omega + (\mathcal{L}(\psi)\,\nabla_{\boldsymbol{\tau}}\psi_k, \mathbf{w}_{\boldsymbol{\tau}})_\Gamma
\end{aligned}
\tag{3.13}
$$

for all $\mathbf{w} \in \mathbb{C}^\infty_{\mathrm{div}}(\overline{\Omega})$, and

$$
\frac{\varphi - \varphi_k}{h} + \mathbf{v}\cdot\nabla\varphi_k = \mathrm{div}\,(m(\varphi_k)\nabla\mu), \qquad \text{almost everywhere in } \Omega, \tag{3.14}
$$

$$
\mu + \frac{c_F}{2}(\varphi + \varphi_k) = -\Delta\varphi + f_0(\varphi) + \sigma\frac{\varphi - \varphi_k}{h}, \qquad \text{almost everywhere in } \Omega, \tag{3.15}
$$

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$$\frac{\psi - \psi_k}{h} + \mathbf{v}_{\boldsymbol{\tau}} \cdot \nabla_{\boldsymbol{\tau}} \psi_k = -l_0\left(\psi_k\right) \mathcal{L}\left(\psi\right), \qquad \text{almost everywhere in } \Gamma, \tag{3.16}$$

$$\mathcal{L}\left(\psi\right) + \frac{c_G}{2}\left(\psi + \psi_k\right) = -\Delta_{\boldsymbol{\tau}} \psi + \partial_{\mathbf{n}} \varphi + \zeta \psi + g_0\left(\psi\right), \qquad \text{almost everywhere in } \Gamma. \tag{3.17}$$

Here, the potentials given by

$$F_0\left(r\right) = F\left(r\right) + \frac{c_F}{2} r^2 \quad \text{and} \quad G_0\left(r\right) = G\left(r\right) + \frac{c_G}{2} r^2 \tag{3.18}$$

are convex functions owing to the assumptions (3.2)–(3.3). In particular,

$$f_0 = F_0' \quad \text{and} \quad g_0 = G_0'.$$

Remark 3.3. Referring to the third term on the right-had side of (3.13), we have discretized (3.10) in the following fashion:

$$\frac{\rho - \rho_k}{h} + \operatorname{div}\left(\rho_k \mathbf{v} + \mathbf{J}\right) = R_{k+1}, \tag{3.19}$$

where $\mathbf{J}$ is given by (3.12). Observe that, thanks to the obvious identity

$$\operatorname{div}(\mathbf{v} \otimes \mathbf{J}) = (\operatorname{div}\mathbf{J})\mathbf{v} + (\mathbf{J} \cdot \nabla)\, \mathbf{v},$$

we can write an equivalent version of (3.13), namely,

$$\begin{aligned}
&\left(\frac{\rho \mathbf{v} - \rho_k \mathbf{v}_k}{h}, \mathbf{w}\right)_\Omega + (\operatorname{div}(\rho_k \mathbf{v} \otimes \mathbf{v}), \mathbf{w})_\Omega + (2\nu(\varphi_k) D\mathbf{v}, D\mathbf{w})_\Omega \\
&\quad + (\beta(\psi_k)\mathbf{v}_{\boldsymbol{\tau}}, \mathbf{w}_{\boldsymbol{\tau}})_\Gamma + \varepsilon\left(|D\mathbf{v}|^{q-2} D\mathbf{v}, D\mathbf{w}\right)_\Omega + \varepsilon\left(|\mathbf{v}|^{q-2}\mathbf{v}, \mathbf{w}\right)_\Omega \\
&\quad + ((\mathbf{J} \cdot \nabla)\, \mathbf{v}, \mathbf{w})_\Omega + \left(\left(\operatorname{div}\mathbf{J} - \frac{\rho - \rho_k}{h} - \mathbf{v} \cdot \nabla \rho_k\right) \frac{\mathbf{v}}{2}, \mathbf{w}\right)_\Omega \\
&= (\mu \nabla \varphi_k, \mathbf{w})_\Omega + \left(\mathcal{L}\left(\psi\right) \nabla_{\boldsymbol{\tau}} \psi_k, \mathbf{w}_{\boldsymbol{\tau}}\right)_\Gamma,
\end{aligned} \tag{3.20}$$

for all $\mathbf{w} \in \mathbb{C}^\infty_{\operatorname{div}}\left(\overline{\Omega}\right)$. In that which follows, we will use (3.20) to deduce a priori estimates for solutions of the time-discrete problem (3.13)–(3.17).

Remark 3.4. Integrating (3.14) with respect to the spatial variable over Ω, using the fact that $\mathbf{v} \in \mathbb{H}^1$, we obtain $\int_\Omega \varphi \mathrm{d}x = \int_\Omega \varphi_k \mathrm{d}x$, which means that

$$\int_\Omega \varphi_k \mathrm{d}x = \int_\Omega \varphi_0 \mathrm{d}x \quad \text{for all } k.$$

Namely, the mass conservation property is also preserved at the discrete level.

For the convenience of notation, we define the following family of Banach spaces

$$\mathbb{U}_\varepsilon := \begin{cases} \mathbb{H}^1, & \text{if } \varepsilon = 0, \\ \mathbb{W}^{1,q}_{\operatorname{div}} = \overline{\mathbb{C}^\infty_{\operatorname{div}}\left(\overline{\Omega}\right)}^{\mathbb{W}^{1,q}(\Omega)} \quad \text{for some } q > 2d, & \text{if } \varepsilon \in (0, 1]. \end{cases}$$

Then the existence of a solution to the time-discrete problem (3.13)–(3.17) is given by

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Lemma 3.3. *Suppose that Assumption 2 is satisfied. Let* $\mathbf{v}_k \in \mathbb{H}$*,* $(\varphi_k, \psi_k) \in V^2$*,* $\sigma, \varepsilon \in [0, 1]$ *and* $\rho_k = \rho(\varphi_k)$ *be given. Then there is some* $(\mathbf{v}, \mu, \varphi, \psi) \in \mathbb{U}_\varepsilon \times H^2_n(\Omega) \times V^2$ *that solves the discrete problem* (3.13)–(3.17) *and in addition, satisfies the following discrete energy inequality:*

$$\begin{aligned}
&E_{\text{tot}}(\mathbf{v}, \varphi, \psi) + \int_\Omega \rho_k \frac{|\mathbf{v}-\mathbf{v}_k|^2}{2} dx + \frac{1}{2}\|(\varphi-\varphi_k, \psi-\psi_k)\|^2_{V^1} \\
&\qquad + h\int_\Omega 2\nu(\varphi_k)|D\mathbf{v}|^2 dx + \varepsilon h \int_\Omega \left(|D\mathbf{v}|^q + |\mathbf{v}|^q\right) dx \\
&\qquad + h\int_\Gamma \beta(\psi_k)\,|\mathbf{v}_\tau|^2\, dS + h\int_\Omega m(\varphi_k)|\nabla\mu|^2 dx \\
&\qquad + h\int_\Gamma l_0(\psi_k)|\mathcal{L}(\psi)|^2 dS + \frac{\sigma}{h}\|\varphi-\varphi_k\|^2_{L^2(\Omega)} \\
&\leqq E_{\text{tot}}(\mathbf{v}_k, \varphi_k, \psi_k).
\end{aligned} \tag{3.21}$$

Remark 3.5. At the discrete level, the presence of any (ε, σ)-terms is in fact not required. In particular, the discretization scheme works for the limiting case $\varepsilon = \sigma = 0$ as well.

Proof. The proof of Lemma 3.3 consists of several steps.

Step 1 (*The discrete energy estimate*). First, we show the a priori estimate (3.21) for any $(\mathbf{v}, \mu, \varphi, \psi) \in \mathbb{U}_\varepsilon \times H^2_n(\Omega) \times V^2$ solving the problem (3.13)–(3.17). In order to test (3.20) with $\mathbf{w} = \mathbf{v}$, we recall the following identities (see for example, [5, Lemma 4.3]):

$$\int_\Omega \left((\text{div}\,\mathbf{J})\frac{\mathbf{v}}{2} + (\mathbf{J}\cdot\nabla)\,\mathbf{v}\right)\cdot\mathbf{v}\text{d}x = \int_\Omega \text{div}\left(\mathbf{J}\frac{|\mathbf{v}|^2}{2}\right)\text{d}x = 0,$$

$$\int_\Omega \left(\text{div}(\rho_k\mathbf{v}\otimes\mathbf{v}) - (\mathbf{v}\cdot\nabla\rho_k)\frac{\mathbf{v}}{2}\right)\cdot\mathbf{v}\text{d}x = \int_\Omega \text{div}\left(\rho_k\mathbf{v}\frac{|\mathbf{v}|^2}{2}\right)\text{d}x = 0.$$

In addition, the algebraic identity

$$\mathbf{a}\cdot(\mathbf{a}-\mathbf{b}) = \frac{|\mathbf{a}|^2}{2} - \frac{|\mathbf{b}|^2}{2} + \frac{|\mathbf{a}-\mathbf{b}|^2}{2} \quad \text{for } \mathbf{a}, \mathbf{b} \in \mathbb{R}^d$$

yields that

$$\frac{1}{h}(\rho\mathbf{v} - \rho_k\mathbf{v}_k)\cdot\mathbf{v} = \frac{1}{h}\left(\rho\frac{|\mathbf{v}|^2}{2} - \rho_k\frac{|\mathbf{v}_k|^2}{2}\right) + \frac{1}{h}(\rho-\rho_k)\frac{|\mathbf{v}|^2}{2} + \frac{1}{h}\rho_k\frac{|\mathbf{v}-\mathbf{v}_k|^2}{2}.$$

Therefore, taking $\mathbf{w} = \mathbf{v}$ in (3.20) and using the above identities we obtain

$$\begin{aligned}
0 &= \int_\Omega \frac{\rho|\mathbf{v}|^2 - \rho_k|\mathbf{v}_k|^2}{2h}\text{d}x + \int_\Omega \rho_k\frac{|\mathbf{v}-\mathbf{v}_k|^2}{2h}\text{d}x + \int_\Omega 2\nu(\varphi_k)|D\mathbf{v}|^2\text{d}x \\
&\quad + \varepsilon\int_\Omega\left(|D\mathbf{v}|^q + |\mathbf{v}|^q\right)\text{d}x + \int_\Gamma \beta(\psi_k)\,|\mathbf{v}_\tau|^2\,\text{d}S - \int_\Omega \mu\,(\nabla\varphi_k\cdot\mathbf{v})\text{d}x \\
&\quad - \int_\Gamma \mathcal{L}(\psi)\,(\nabla_\tau\psi_k\cdot\mathbf{v}_\tau)\,\text{d}S.
\end{aligned} \tag{3.22}$$

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Moreover, taking μ as a test function for (3.14), we get

$$0=\int_\Omega \frac{\varphi-\varphi_k}{h}\mu \mathrm{d}x+\int_\Omega (\mathbf{v}\cdot\nabla\varphi_k)\mu \mathrm{d}x+\int_\Omega m(\varphi_k)|\nabla\mu|^2\mathrm{d}x. \tag{3.23}$$

Next, we test (3.15) and (3.17) by $\frac{1}{h}(\varphi-\varphi_k)$ and $\frac{1}{h}(\psi-\psi_k)$, respectively. This gives

$$\begin{aligned}0=&\frac{1}{h}\int_\Omega \nabla\varphi\cdot\nabla(\varphi-\varphi_k)\mathrm{d}x+\int_\Omega f_0(\varphi)\frac{1}{h}(\varphi-\varphi_k)\mathrm{d}x\\&-\int_\Gamma \partial_{\mathbf{n}}\varphi\frac{\psi-\psi_k}{h}\mathrm{d}S-\int_\Omega \mu\frac{\varphi-\varphi_k}{h}\mathrm{d}x\\&-\int_\Omega c_F\frac{\varphi^2-\varphi_k^2}{2h}\mathrm{d}x+\sigma\int_\Omega\left(\frac{\varphi-\varphi_k}{h}\right)^2\mathrm{d}x\end{aligned} \tag{3.24}$$

and

$$\begin{aligned}0=&\frac{1}{h}\int_\Gamma \nabla_{\boldsymbol{\tau}}\psi\cdot\nabla_{\boldsymbol{\tau}}(\psi-\psi_k)\mathrm{d}S+\frac{\zeta}{h}\int_\Gamma\psi(\psi-\psi_k)\mathrm{d}S+\int_\Gamma\partial_{\mathbf{n}}\varphi\frac{\psi-\psi_k}{h}\mathrm{d}S\\&+\int_\Gamma g_0(\psi)\frac{1}{h}(\psi-\psi_k)\mathrm{d}S-\int_\Gamma c_G\frac{\psi^2-\psi_k^2}{2h}\mathrm{d}S.\end{aligned} \tag{3.25}$$

Finally, testing (3.16) by $-\mathcal{L}(\psi)$, we find

$$0=\int_\Gamma l_0(\psi_k)|\mathcal{L}(\psi)|^2\mathrm{d}S+\int_\Gamma\mathcal{L}(\psi)(\mathbf{v}_{\boldsymbol{\tau}}\cdot\nabla_{\boldsymbol{\tau}}\psi_k)\mathrm{d}S+\int_\Gamma\mathcal{L}(\psi)\frac{\psi-\psi_k}{h}\mathrm{d}S. \tag{3.26}$$

Summing the identities (3.22)–(3.26) together, we obtain

$$\begin{aligned}0=&\int_\Omega\frac{\rho|\mathbf{v}|^2-\rho_k|\mathbf{v}_k|^2}{2h}\mathrm{d}x+\int_\Omega\rho_k\frac{|\mathbf{v}-\mathbf{v}_k|^2}{2h}\mathrm{d}x+\int_\Omega 2\nu(\varphi_k)|D\mathbf{v}|^2\mathrm{d}x\\&+\int_\Gamma\beta(\psi_k)|\mathbf{v}_\tau|^2\mathrm{d}S+\varepsilon\int_\Omega\left(|D\mathbf{v}|^q+|\mathbf{v}|^q\right)\mathrm{d}x+\int_\Omega m(\varphi_k)|\nabla\mu|^2\mathrm{d}x\\&+\int_\Gamma l_0(\psi_k)|\mathcal{L}(\psi)|^2\mathrm{d}S+\int_\Omega f_0(\varphi)\frac{1}{h}(\varphi-\varphi_k)\mathrm{d}x-\int_\Omega c_F\frac{\varphi^2-\varphi_k^2}{2h}\mathrm{d}x\\&+\int_\Gamma g_0(\psi)\frac{1}{h}(\psi-\psi_k)\mathrm{d}S-\int_\Gamma c_G\frac{\psi^2-\psi_k^2}{2h}\mathrm{d}S+\sigma\int_\Omega\left(\frac{\varphi-\varphi_k}{h}\right)^2\mathrm{d}x\\&+\frac{1}{h}\int_\Omega\nabla\varphi\cdot\nabla(\varphi-\varphi_k)\mathrm{d}x+\frac{1}{h}\int_\Gamma\nabla_{\boldsymbol{\tau}}\psi\cdot\nabla_{\boldsymbol{\tau}}(\psi-\psi_k)\mathrm{d}S\\&+\frac{\zeta}{h}\int_\Gamma\psi(\psi-\psi_k)\mathrm{d}S\\\geqq&\int_\Omega\frac{\rho|\mathbf{v}|^2-\rho_k|\mathbf{v}_k|^2}{2h}\mathrm{d}x+\int_\Omega\rho_k\frac{|\mathbf{v}-\mathbf{v}_k|^2}{2h}\mathrm{d}x+\int_\Omega 2\nu(\varphi_k)|D\mathbf{v}|^2\mathrm{d}x\\&+\int_\Gamma\beta(\psi_k)|\mathbf{v}_\tau|^2\mathrm{d}S+\int_\Omega m(\varphi_k)|\nabla\mu|^2\mathrm{d}x+\int_\Gamma l_0(\psi_k)|\mathcal{L}(\psi)|^2\mathrm{d}S\end{aligned}$$

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$$
\begin{aligned}
&+\frac{1}{h}\int_\Omega F_0(\varphi)-F_0(\varphi_k)\mathrm{d}x-\int_\Omega c_F\frac{\varphi^2-\varphi_k^2}{2h}\mathrm{d}x\\
&+\frac{1}{h}\int_\Gamma G_0(\psi)-G_0\left(\psi_k\right)\mathrm{d}S-\int_\Gamma c_G\frac{\psi^2-\psi_k^2}{2h}\mathrm{d}S\\
&+\frac{1}{h}\|(\varphi-\varphi_k,\psi-\psi_k)\|_{V^1}^2+\sigma\int_\Omega\left(\frac{\varphi-\varphi_k}{h}\right)^2\mathrm{d}x\\
&+\frac{1}{h}\int_\Omega\frac{|\nabla\varphi|^2}{2}-\frac{|\nabla\varphi_k|^2}{2}\mathrm{d}x+\frac{1}{h}\int_\Gamma\frac{|\nabla_{\boldsymbol{\tau}}\psi|^2}{2}-\frac{|\nabla_{\boldsymbol{\tau}}\psi_k|^2}{2}\mathrm{d}S\\
&+\frac{\zeta}{h}\int_\Gamma\frac{|\psi|^2}{2}-\frac{|\psi_k|^2}{2}\mathrm{d}S,
\end{aligned}
\tag{3.27}
$$

where we have used the inequalities (recall that $F_0,\ G_0$ are convex functions)

$$
f_0(\varphi)\,(\varphi-\varphi_k)\geqq F_0(\varphi)-F_0(\varphi_k),\quad g_0(\psi)\,(\psi-\psi_k)\geqq G_0(\psi)-G_0(\psi_k)
\tag{3.28}
$$

as well as the identities

$$
\nabla\varphi\cdot\nabla(\varphi-\varphi_k)=\frac{|\nabla\varphi|^2}{2}-\frac{|\nabla\varphi_k|^2}{2}+\frac{|\nabla\varphi-\nabla\varphi_k|^2}{2},
\tag{3.29}
$$

$$
\nabla_{\boldsymbol{\tau}}\psi\cdot\nabla_{\boldsymbol{\tau}}(\psi-\psi_k)=\frac{|\nabla_{\boldsymbol{\tau}}\psi|^2}{2}-\frac{|\nabla_{\boldsymbol{\tau}}\psi_k|^2}{2}+\frac{|\nabla_{\boldsymbol{\tau}}\psi-\nabla_{\boldsymbol{\tau}}\psi_k|^2}{2}.
\tag{3.30}
$$

Then we immediately obtain the claimed discrete energy estimate (3.21) from (3.27) and the definition of E_{tot} (recall (2.23)).

Step 2 (*The fixed point argument*). In order to show the existence of a weak solution to the discrete problem (3.13)–(3.17), we apply the Leray–Schauder principle. To this end, we define the nonlinear operators $\mathcal{M}_k,\ \mathcal{F}_k:\ X\to Y$, where

$$
X=\mathbb{U}_\varepsilon\times H_n^2(\Omega)\times V^2,\quad Y=(\mathbb{U}_\varepsilon)^*\times L^2(\Omega)\times\left(L^2(\Omega)\times L^2\left(\Gamma\right)\right).
$$

More precisely, for $\mathbf{p}=(\mathbf{v},\mu,\varphi,\psi)\in X$, we set

$$
\mathcal{M}_k(\mathbf{p})=\begin{pmatrix} L_{k,\varepsilon}(\mathbf{v})\\ -\mathrm{div}(m(\varphi_k)\nabla\mu)+\int_\Omega\mu\mathrm{d}x\\ A_W\begin{pmatrix}\varphi\\ \psi\end{pmatrix}\end{pmatrix},
$$

where

$$
\begin{aligned}
\left\langle L_{k,\varepsilon}(\mathbf{v}),\mathbf{w}\right\rangle&=\varepsilon\int_\Omega|D\mathbf{v}|^{q-2}D\mathbf{v}:D\mathbf{w}\mathrm{d}x+\varepsilon\int_\Omega|\mathbf{v}|^{q-2}\mathbf{v}\cdot\mathbf{w}\mathrm{d}x\\
&\quad+\int_\Omega 2\nu(\varphi_k)D\mathbf{v}:D\mathbf{w}\mathrm{d}x+\int_\Gamma\beta(\psi_k)\mathbf{v}_{\boldsymbol{\tau}}\cdot\mathbf{w}_{\boldsymbol{\tau}}\mathrm{d}S,
\end{aligned}
$$

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for all $\mathbf{w} \in \mathbb{U}_\varepsilon$, while the operator A_W denotes the so-called *Wentzell* Laplacian (see, for example, [30]), given by

$$A_W \begin{pmatrix} \varphi \\ \psi \end{pmatrix} = \begin{pmatrix} -\Delta\varphi \\ -\Delta_{\boldsymbol{\tau}}\psi + \partial_{\mathbf{n}}\varphi + \zeta\psi \end{pmatrix}, \quad \begin{pmatrix} \varphi \\ \psi \end{pmatrix} \in \mathrm{dom}\,(A_W) = V^2.$$

Note that since $\zeta > 0$, A_W is positive and for any $(\varphi, \psi) \in \mathrm{dom}\,(A_W)$, it holds $A_W \begin{pmatrix} \varphi \\ \psi \end{pmatrix} \in L^2(\Omega) \times L^2(\Gamma)$. Therefore, the last line in $\mathcal{M}_k(\mathbf{p})$ lies in $L^2(\Omega) \times L^2(\Gamma)$. Furthermore, for $\mathbf{p} = (\mathbf{v}, \mu, \Xi) \in X$ with $\Xi := \begin{pmatrix} \varphi \\ \psi \end{pmatrix}$, we define

$$\mathcal{F}_k(\mathbf{p}) = \begin{pmatrix} \mathbf{S}_\Omega + \mathbf{S}_\Gamma \\ -\dfrac{\varphi - \varphi_k}{h} - \mathbf{v} \cdot \nabla\varphi_k + \displaystyle\int_\Omega \mu \mathrm{d}x \\ \begin{pmatrix} \mu + \dfrac{c_F}{2}(\varphi + \varphi_k) - f_0(\varphi) - \dfrac{\sigma}{h}(\varphi - \varphi_k) \\ \mathcal{L}(\psi) + \dfrac{c_G}{2}(\psi + \psi_k) - g_0(\psi) \end{pmatrix} \end{pmatrix},$$

where

$$\begin{aligned} \mathbf{S}_\Omega &:= -\frac{\rho\mathbf{v} - \rho_k\mathbf{v}_k}{h} - \mathrm{div}(\rho_k\mathbf{v} \otimes \mathbf{v}) + \mu\nabla\varphi_k \\ &\quad - \left(\mathrm{div}\mathbf{J} - \frac{\rho - \rho_k}{h} - \mathbf{v} \cdot \nabla\rho_k\right)\frac{\mathbf{v}}{2} - (\mathbf{J} \cdot \nabla)\,\mathbf{v}, \\ \mathbf{S}_\Gamma &:= \mathcal{L}(\psi)\,\nabla_{\boldsymbol{\tau}}\psi_k. \end{aligned}$$

In particular, the first line $\mathcal{F}_k^{(1)}(\mathbf{p})$ of $\mathcal{F}_k(\mathbf{p})$ must be understood as follows:

$$\left\langle \mathcal{F}_k^{(1)}(\mathbf{p}), \mathbf{w} \right\rangle = \int_\Omega \mathbf{S}_\Omega \cdot \mathbf{w}\,\mathrm{d}x + \int_\Gamma \mathbf{S}_\Gamma \cdot \mathbf{w}_{\boldsymbol{\tau}}\,\mathrm{d}S, \quad \text{for all } \mathbf{w} \in \mathbb{U}_\varepsilon \subseteq \mathbb{H}^1.$$

The remaining lines of $\mathcal{F}_k(\mathbf{p})$ are defined in a pointwise sense (that is, almost everywhere). Besides, in the last line of $\mathcal{F}_k(\mathbf{p})$, $\mathcal{L}(\psi)$ also satisfies the following equation pointwisely almost everywhere

$$\mathcal{L}(\psi) = -\frac{1}{l_0(\psi_k)}\left(\frac{\psi - \psi_k}{h} + \mathbf{v}_{\boldsymbol{\tau}} \cdot \nabla_{\boldsymbol{\tau}}\psi_k\right). \tag{3.31}$$

Then $\mathbf{p} = (\mathbf{v}, \mu, \varphi, \psi) \in X$ is a weak solution of the time discrete problem (3.13)–(3.17) *if and only if*

$$\mathcal{M}_k(\mathbf{p}) = \mathcal{F}_k(\mathbf{p}).$$

Note that here we have used the equivalent version (3.20) instead of (3.13).

The standard theory of partial differential equations implies the invertibility of $L_{k,\varepsilon} : \mathbb{U}_\varepsilon \to (\mathbb{U}_\varepsilon)^*$ and the continuity of $L_{k,\varepsilon}^{-1}$. Indeed, $L_{k,\varepsilon}$ is a strictly monotone operator, namely,

$$\left\langle L_{k,\varepsilon}\mathbf{v} - L_{k,\varepsilon}\mathbf{w}, \mathbf{v} - \mathbf{w} \right\rangle \geqq 0, \quad \forall\, \mathbf{v},\ \mathbf{w} \in \mathbb{U}_\varepsilon$$

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and

$$\langle L_{k,\varepsilon}\mathbf{v} - L_{k,\varepsilon}\mathbf{w},\ \mathbf{v} - \mathbf{w}\rangle = 0, \quad \text{if and only if } \mathbf{v} = \mathbf{w}.$$

Moreover, the operator $L_{k,\varepsilon}$ is clearly coercive (and thus onto) since

$$\lim_{\|\mathbf{v}\|_{\mathbb{U}_\varepsilon}\to+\infty} \frac{\langle L_{k,\varepsilon}\mathbf{v}, \mathbf{v}\rangle}{\|\mathbf{v}\|_{\mathbb{U}_\varepsilon}} = +\infty. \tag{3.32}$$

Hence, it follows that $L_{k,\varepsilon}$ is a bijection. To show the continuity of its inverse $L_{k,\varepsilon}^{-1}$, if $\mathbf{w}_n \to \mathbf{w}$ in $(\mathbb{U}_\varepsilon)^*$ such that $L_{k,\varepsilon}\mathbf{v}_n = \mathbf{w}_n$ and $L_{k,\varepsilon}\mathbf{v} = \mathbf{w}$, then by the boundedness of $\mathbf{w}_n$ in $(\mathbb{U}_\varepsilon)^*$ and (3.32), we have

$$\langle L_{k,\varepsilon}\mathbf{v}_n - L_{k,\varepsilon}\mathbf{v},\ \mathbf{v}_n - \mathbf{v}\rangle = \langle \mathbf{w}_n - \mathbf{w}, \mathbf{v}_n - \mathbf{v}\rangle \to 0$$

since $\mathbf{w}_n \to \mathbf{w}$ (in the strong sense). It follows in the least that $\mathbf{v}_n \to \mathbf{v}$ (strongly) in $\mathbb{U}_0$ for any $\varepsilon \in [0, 1]$. Since $\mathbf{v}_n$ is bounded in $\mathbb{U}_\varepsilon$, then it also holds $\mathbf{v}_n \rightharpoonup \mathbf{v}$ (weakly) in $\mathbb{U}_\varepsilon$ for $\varepsilon > 0$. Finally, for each $\varepsilon > 0$, since

$$\varepsilon \limsup_{n\to\infty} \|\mathbf{v}_n\|^q_{\mathbb{W}^{1,q}} \leqq \limsup_{n\to\infty} \langle L_{k,\varepsilon}\mathbf{v}_n, \mathbf{v}_n\rangle = \langle L_{k,\varepsilon}\mathbf{v}, \mathbf{v}\rangle \leqq \varepsilon \|\mathbf{v}\|^q_{\mathbb{W}^{1,q}},$$

we can deduce that $\mathbf{v}_n \to \mathbf{v}$ (strongly) in $\mathbb{U}_\varepsilon$ for $\varepsilon > 0$ as well.

Following [5], we consider for a given function $\alpha \in L^2(\Omega)$ the elliptic boundary value problem

$$\begin{cases} -\mathrm{div}(m(\varphi_k)\nabla\mu) + \int_\Omega \mu \mathrm{d}x = \alpha, & \text{in } \Omega, \\ \partial_{\mathbf{n}}\mu = 0, & \text{on } \Gamma. \end{cases}$$

There exists a unique weak solution $\mu \in H^2_n(\Omega)$ satisfying the estimate

$$\|\mu\|_{H^2(\Omega)} \leqq C_k \left(\|\mu\|_{H^1(\Omega)} + \|\alpha\|_{L^2(\Omega)}\right) \tag{3.33}$$

for some positive constant $C_k = C_k\left(\|\varphi_k\|_{L^\infty(\Omega)}\right)$.

Besides, since the Wentzell Laplacian A_W is positive and linear, the operator $A_W : V^2 \to L^2(\Omega) \times L^2(\Gamma)$ is invertible and A_W^{-1} is continuous as a mapping from $L^2(\Omega) \times L^2(\Gamma)$ into V^2 (see [30]).

In summary, we obtain that the operator $\mathcal{M}_k : X \to Y$ is invertible with a continuous inverse $\mathcal{M}_k^{-1} : Y \to X$. To further get a compact operator, we introduce the Banach space

$$\widetilde{Y} := \left(\mathbb{H}^{3/4}\right)^* \times W^{1,3/2}(\Omega) \times \left(W^{1/2,2}(\Omega) \times W^{1/4,2}(\Gamma)\right).$$

Since $\widetilde{Y} \overset{c}{\hookrightarrow} Y$ due to $\mathbb{U}_\varepsilon \overset{c}{\hookrightarrow} \mathbb{H}^{3/4}$, the restriction $\mathcal{M}_k^{-1} : \widetilde{Y} \subset Y \to X$ is indeed a compact operator.

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The next step is to show that the operator $\mathcal{F}_k : X \to \widetilde{Y}$ is continuous and it maps bounded sets into bounded sets. More precisely, we have the following estimates (note that $(\varphi_k, \psi_k) \in V^2$ and therefore $\rho_k \in H^2(\Omega)$):

$$
\begin{aligned}
&\|\rho \mathbf{v}\|_{\mathbb{H}^{-3/4}(\Omega)} \leqq C\|\mathbf{v}\|_{\mathbb{H}^1(\Omega)}(\|\varphi\|_{L^2(\Omega)}+1),\\
&\|\mathrm{div}(\rho_k \mathbf{v}\otimes \mathbf{v})\|_{\mathbb{H}^{-3/4}(\Omega)} \leqq C_k\|\mathbf{v}\|^2_{\mathbb{H}^1(\Omega)},\\
&\|\mu\nabla\varphi_k\|_{\mathbb{H}^{-3/4}(\Omega)} \leqq C_k\|\mu\|_{L^2(\Omega)},\\
&\|(\mathrm{div}\mathbf{J})\mathbf{v}\|_{\mathbb{H}^{-3/4}(\Omega)} \leqq C_k\|\mathbf{v}\|_{\mathbb{H}^1(\Omega)}\|\mu\|_{H^2(\Omega)},\\
&\|(\mathbf{J}\cdot\nabla)\mathbf{v}\|_{\mathbb{H}^{-3/4}(\Omega)} \leqq C\|\mathbf{v}\|_{\mathbb{H}^1(\Omega)}\|\mu\|_{H^2(\Omega)},\\
&\|\mathbf{v}\cdot\nabla\varphi_k\|_{W^{1,3/2}(\Omega)} \leqq C_k\|\mathbf{v}\|_{\mathbb{H}^1(\Omega)},\\
&\|\mathbf{v}_{\boldsymbol{\tau}}\cdot\nabla_{\boldsymbol{\tau}}\psi_k\|_{W^{1/4,2}(\Gamma)} \leqq C_k\,\|\mathbf{v}\|_{\mathbb{H}^1(\Omega)}\,.
\end{aligned}
$$

The first six estimates follow directly from [5, (i)–(vi), pp. 467], using the fact that $L^{3/2}(\Omega) \hookrightarrow \left(H^{3/4}(\Omega)\right)^* := H^{-3/4}(\Omega)$. Note that $f_0(\cdot)$ as a nonlinear mapping from $H^2(\Omega) \to W^{1/2,2}(\Omega)$ is continuous and maps bounded sets to bounded sets, due to the growth assumption in (3.3). Analogously, the same conclusion holds for the nonlinear mapping $g_0(\cdot) : H^2(\Gamma) \to W^{1/4,2}(\Gamma)$. In the seventh estimate involving $\mathbf{v}_{\boldsymbol{\tau}}\cdot\nabla_{\boldsymbol{\tau}}\psi_k$, we have exploited the fact that $\mathbf{v}_{\tau_j}\partial_{\tau_j}\psi$ is bounded in $W^{1/4,2}(\Gamma)$, as a product of functions in $W^{1/2,2}(\Gamma)\times H^1(\Gamma)$ (cf. Lemma B.3). Next, recalling the definition of $\mathbf{S}_\Gamma$, we also have

$$
\sup_{\|\mathbf{w}\|_{\mathbb{H}^{3/4}}\leqq 1} |(\mathbf{S}_\Gamma,\, \mathbf{w}_{\boldsymbol{\tau}})_\Gamma| \leqq C_k\,\|\mathcal{L}(\psi)\|_{H^{1/4}(\Gamma)}\,,
$$

where $\mathcal{L}(\psi)$, as defined pointwisely in (3.31) in terms of $(\psi, \mathbf{v})$, is a continuous operator from $H^2(\Gamma)\times\mathbb{H}^1 \to W^{1/4,2}(\Gamma)$, mapping bounded subsets to bounded subsets. More precisely, according to Lemma B.3 (for some $\varepsilon\in(0,1/8)$), we have

$$
\begin{aligned}
\|\mathcal{L}(\psi)\|_{H^{1/4}(\Gamma)} &\leqq \|1/l_0(\psi_k)\|_{L^2(\Gamma)}\,\|(\psi-\psi_k)/h\|_{H^2(\Gamma)}\\
&\quad+\|1/l_0(\psi_k)\|_{W^{3/4+2\varepsilon,2}(\Gamma)}\,\|\mathbf{v}_{\boldsymbol{\tau}}\cdot\nabla_{\boldsymbol{\tau}}\psi_k\|_{W^{1/2-\varepsilon,2}(\Gamma)}\\
&\leqq C_k\left(\|\psi\|_{H^2(\Gamma)}+\|\mathbf{v}\|_{\mathbb{H}^1(\Omega)}+1\right).
\end{aligned}
$$

In order to apply the Leray–Schauder principle on $\widetilde{Y}$, we rewrite the identity $\mathcal{M}_k(\mathbf{p}) = \mathcal{F}_k(\mathbf{p})$ for a solution $\mathbf{p}\in X$ of problem (3.13)–(3.17) into the following form:

$$
\left(\mathcal{F}_k\circ\mathcal{M}_k^{-1}\right)(\mathbf{f}) = \mathbf{f}, \quad \text{for } \mathbf{f} = \mathcal{M}_k(\mathbf{p})\,.
$$

Note that the mapping $\mathcal{K}_k := \mathcal{F}_k\circ\mathcal{M}_k^{-1} : \widetilde{Y}\to\widetilde{Y}$ is a compact operator because $\mathcal{M}_k^{-1}$ is compact and $\mathcal{F}_k$ is continuous. The foregoing equation is then equivalent to finding a fixed point of $\mathcal{K}_k$, namely,

$$
\mathcal{K}_k(\mathbf{f}) = \mathbf{f}.
$$

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The existence of such a fixed point can be deduced by an application of the abstract result [74, Theorem 6.A], where it remains to show that

$$\exists\, R>0 \textit{ such that, if } \mathbf{f}\in\widetilde{Y} \textit{ and } 0\leqq\lambda\leqq 1 \textit{ fulfill } \mathbf{f}=\lambda\mathcal{K}_k\left(\mathbf{f}\right), \textit{ then } \|\mathbf{f}\|_{\widetilde{Y}}\leqq R. \tag{3.34}$$

For this purpose, let $\mathbf{f}\in\widetilde{Y}$ and $0\leqq\lambda\leqq 1$ satisfying $\mathbf{f}=\lambda\mathcal{K}_k\left(\mathbf{f}\right)$. With $\mathbf{p}=\mathcal{M}_k^{-1}(\mathbf{f})$ we have

$$\mathbf{f}=\lambda\mathcal{K}_k(\mathbf{f}) \quad\Longleftrightarrow\quad \mathcal{M}_k(\mathbf{p})-\lambda\mathcal{F}_k(\mathbf{p})=0, \tag{3.35}$$

which is equivalent to the weak formulation

$$\begin{aligned}
&\varepsilon\int_\Omega |D\mathbf{v}|^{q-2}\,D\mathbf{v}:D\mathbf{w}\mathrm{d}x+\varepsilon\int_\Omega|\mathbf{v}|^{q-2}\,\mathbf{v}\cdot\mathbf{w}\mathrm{d}x+\int_\Omega 2\nu(\varphi_k)D\mathbf{v}:D\mathbf{w}\mathrm{d}x\\
&\quad+\int_\Gamma\beta(\psi_k)\mathbf{v}_{\boldsymbol{\tau}}\cdot\mathbf{w}_{\boldsymbol{\tau}}\mathrm{d}S+\lambda\int_\Omega\frac{\rho\mathbf{v}-\rho_k\mathbf{v}_k}{h}\cdot\mathbf{w}\mathrm{d}x\\
&\quad+\lambda\int_\Omega\mathrm{div}(\rho_k\mathbf{v}\otimes\mathbf{v})\cdot\mathbf{w}\mathrm{d}x+\lambda\int_\Omega\left(\mathrm{div}\mathbf{J}-\frac{\rho-\rho_k}{h}-\mathbf{v}\cdot\nabla\rho_k\right)\frac{\mathbf{v}}{2}\cdot\mathbf{w}\mathrm{d}x\\
&\quad+\lambda\int_\Omega\left(\mathbf{J}\cdot\nabla\right)\mathbf{v}\cdot\mathbf{w}\mathrm{d}x\\
&=\lambda\int_\Omega\mu\left(\nabla\varphi_k\cdot\mathbf{w}\right)\mathrm{d}x+\lambda\int_\Gamma\mathcal{L}\left(\psi\right)\left(\mathbf{w}_{\boldsymbol{\tau}}\cdot\nabla_{\boldsymbol{\tau}}\psi_k\right)\mathrm{d}S,
\end{aligned}\tag{3.36}$$

for all $\mathbf{w}\in\mathbb{U}_\varepsilon$, and the pointwise identities

$$\begin{cases}
\mathrm{div}(m(\varphi_k)\nabla\mu)-\int_\Omega\mu\mathrm{d}x=\lambda\dfrac{\varphi-\varphi_k}{h}+\lambda\mathbf{v}\cdot\nabla\varphi_k-\lambda\int_\Omega\mu\mathrm{d}x,\\
-\Delta\varphi=\lambda\mu+\lambda\dfrac{c_F}{2}\left(\varphi+\varphi_k\right)-\lambda f_0\left(\varphi\right)-\lambda\sigma\dfrac{\varphi-\varphi_k}{h},\\
-\Delta_{\boldsymbol{\tau}}\psi+\partial_{\mathbf{n}}\varphi+\zeta\psi=\lambda\mathcal{L}\left(\psi\right)+\lambda\dfrac{c_G}{2}\left(\psi+\psi_k\right)-\lambda g_0\left(\psi\right),
\end{cases}\tag{3.37}$$

for $\mu\in H_n^2\left(\Omega\right)$, $(\varphi,\psi)\in V^2$, with $\mathcal{L}\left(\psi\right)$ being given pointwisely by (3.31).

Analogously as in the derivation of the discrete energy estimate (3.21), we set $\mathbf{w}=\mathbf{v}$ in (3.36), test the first equation of (3.37) with μ, the second and third ones of (3.37) with $\frac{1}{h}(\varphi-\varphi_k)$ and $\frac{1}{h}\left(\psi-\psi_k\right)$, respectively. Similar calculations yield that

$$\begin{aligned}
&\lambda\int_\Omega\frac{\rho|\mathbf{v}|^2-\rho_k|\mathbf{v}_k|^2}{2h}\mathrm{d}x+\lambda\int_\Omega\rho_k\frac{|\mathbf{v}-\mathbf{v}_k|^2}{2h}\mathrm{d}x+\varepsilon\int_\Omega\left(|D\mathbf{v}|^q+|\mathbf{v}|^q\right)\mathrm{d}x\\
&\quad+\int_\Omega 2\nu(\varphi_k)|D\mathbf{v}|^2\mathrm{d}x+\int_\Gamma\beta(\psi_k)\left|\mathbf{v}_{\boldsymbol{\tau}}\right|^2\mathrm{d}S+\int_\Omega m(\varphi_k)|\nabla\mu|^2\mathrm{d}x\\
&\quad+\lambda\int_\Gamma l_0\left(\psi_k\right)\left|\mathcal{L}\left(\psi\right)\right|^2\mathrm{d}S+\frac{\lambda}{h}\int_\Omega f_0(\varphi)(\varphi-\varphi_k)\mathrm{d}x\\
&\quad+\frac{\lambda}{h}\int_\Gamma g_0(\psi)(\psi-\psi_k)\mathrm{d}S+(1-\lambda)\left(\int_\Omega\mu\mathrm{d}x\right)^2\\
&\quad+\lambda\sigma\int_\Omega\left(\frac{\varphi-\varphi_k}{h}\right)^2\mathrm{d}x+\frac{1}{h}\int_\Omega\nabla\varphi\cdot\nabla(\varphi-\varphi_k)\mathrm{d}x
\end{aligned}$$

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$$+\frac{1}{h}\int_\Gamma \nabla_{\boldsymbol{\tau}}\psi\cdot\nabla_{\boldsymbol{\tau}}(\psi-\psi_k)\mathrm{d}S+\frac{\zeta}{h}\int_\Gamma \psi(\psi-\psi_k)\mathrm{d}S$$
$$=\lambda c_F\int_\Omega \frac{\varphi^2-\varphi_k^2}{2h}\mathrm{d}x+\lambda c_G\int_\Gamma \frac{\psi^2-\psi_k^2}{2h}\mathrm{d}S. \tag{3.38}$$

Exploiting now the inequality (3.28) and the identities (3.29)–(3.30) once again, dropping any non-essential nonnegative terms on the left-hand side, we deduce the inequality

$$\begin{aligned}
&\lambda\int_\Omega \frac{\rho|\mathbf{v}|^2}{2}\mathrm{d}x+\lambda\int_\Omega \rho_k\frac{|\mathbf{v}-\mathbf{v}_k|^2}{2}\mathrm{d}x+h\varepsilon\int_\Omega\left(|D\mathbf{v}|^q+|\mathbf{v}|^q\right)\mathrm{d}x\\
&\quad+h\int_\Omega 2\nu(\varphi_k)|D\mathbf{v}|^2\mathrm{d}x+h\int_\Gamma \beta(\psi_k)\,|\mathbf{v}_{\boldsymbol{\tau}}|^2\,\mathrm{d}S\\
&\quad+h\int_\Omega m(\varphi_k)|\nabla\mu|^2\mathrm{d}x+\lambda h\int_\Gamma l_0\left(\psi_k\right)|\mathcal{L}\left(\psi\right)|^2\,\mathrm{d}S\\
&\quad+(1-\lambda)\,h\left(\int_\Omega\mu\mathrm{d}x\right)^2+\lambda\sigma h\int_\Omega\left(\frac{\varphi-\varphi_k}{h}\right)^2\mathrm{d}x\\
&\quad+\frac{1}{2}\left\|(\varphi,\psi)\right\|_{V^1}^2+\lambda\int_\Omega\left(F_0(\varphi)-\frac{c_F}{2}\varphi^2\right)\mathrm{d}x\\
&\quad+\lambda\int_\Gamma\left(G_0(\psi)-\frac{c_G}{2}\psi^2\right)\mathrm{d}S\\
&\leqq\lambda\int_\Omega\frac{\rho_k|\mathbf{v}_k|^2}{2}\mathrm{d}x+\frac{1}{2}\left\|(\varphi_k,\psi_k)\right\|_{V^1}^2+\lambda\int_\Omega\left(F_0\left(\varphi_k\right)-\frac{c_F}{2}\varphi_k^2\right)\mathrm{d}x\\
&\quad+\lambda\int_\Gamma\left(G_0(\psi_k)-\frac{c_G}{2}\psi_k^2\right)\mathrm{d}S.
\end{aligned}\tag{3.39}$$

In order to absorb the potentially nonnegative quadratic terms on the left-hand side of (3.39), we recall (3.18) and the assumptions (3.2)–(3.3) to deduce that

$$\lambda\int_\Omega\left(F_0(\varphi)-\frac{c_F}{2}\varphi^2\right)\mathrm{d}x=\lambda\int_\Omega F(\varphi)\mathrm{d}x\geqq-\lambda c_F\,|\Omega|\,, \tag{3.40}$$
$$\lambda\int_\Gamma\left(G_0(\psi)-\frac{c_G}{2}\psi^2\right)\mathrm{d}S=\lambda\int_\Gamma G(\psi)\mathrm{d}S\geqq-\lambda c_G\,|\Gamma|\,. \tag{3.41}$$

Then by ignoring certain summands that have a factor λ or $1-\lambda$ (since they do not give a contribution to some estimates of $\|\mathbf{p}\|_X$ independent of $\lambda\in[0,1]$), we infer from (3.39)–(3.41) that

$$\begin{aligned}
&h\int_\Omega 2\nu(\varphi_k)|D\mathbf{v}|^2\mathrm{d}x+h\int_\Gamma\beta(\psi_k)\,|\mathbf{v}_{\boldsymbol{\tau}}|^2\,\mathrm{d}S+h\int_\Omega m(\varphi_k)|\nabla\mu|^2\mathrm{d}x\\
&\quad+\frac{1}{2}\left\|(\varphi,\psi)\right\|_{V^1}^2+h\varepsilon\int_\Omega\left(|D\mathbf{v}|^q+|\mathbf{v}|^q\right)\mathrm{d}x\\
&\quad+\lambda\sigma\int_\Omega\frac{(\varphi-\varphi_k)^2}{h}\mathrm{d}x+(1-\lambda)\,h\left(\int_\Omega\mu\mathrm{d}x\right)^2
\end{aligned}$$

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$$
\begin{aligned}
&+\lambda h\int_\Gamma l_0\left(\psi_k\right)\left|\mathcal{L}\left(\psi\right)\right|^2 \mathrm{d}S \\
&\leqq C_k. \qquad (3.42)
\end{aligned}
$$

Korn's inequality for $\mathbf{v}\in\mathbb{U}_\varepsilon$ and the fact that ν, β, l_0 and m are all bounded from below by certain positive constants, gives the following bound:

$$
\begin{aligned}
&\|\mathbf{v}\|_{\mathbb{H}^1(\Omega)}+\varepsilon^{1/q}\|\mathbf{v}\|_{\mathbb{W}^{1,q}(\Omega)}+\|\nabla\mu\|_{L^2(\Omega)}+\|(\varphi,\psi)\|_{V^1}\\
&\quad+\sqrt{1-\lambda}\left|\int_\Omega\mu\mathrm{d}x\right|+\sqrt{\lambda}\left\|\mathcal{L}\left(\psi\right)\right\|_{L^2(\Gamma)}\\
&\leqq C_k, \qquad (3.43)
\end{aligned}
$$

where the constant C_k depends on h but is independent of λ.

To get an estimate on the L^2-norm of the chemical potential μ, we distinguish two cases. For $\lambda\in[0,\frac12)$, we directly use (3.43) to obtain $\left|\int_\Omega\mu\mathrm{d}x\right|\leqq C_k$. For $\lambda\in[\frac12,1]$, we integrate the pointwise identities associated with the last two lines of (3.37) to get

$$
\begin{aligned}
\lambda\int_\Omega\mu\mathrm{d}x&=\lambda\int_\Omega f_0\left(\varphi\right)\mathrm{d}x-\lambda\frac{c_F}{2}\int_\Omega\left(\varphi+\varphi_k\right)\mathrm{d}x+\zeta\int_\Gamma\psi\mathrm{d}S\\
&\quad+\lambda\sigma\int_\Omega\frac{\varphi-\varphi_k}{h}\mathrm{d}x+\lambda\int_\Gamma g_0\left(\psi\right)\mathrm{d}S\\
&\quad-\lambda\frac{c_G}{2}\int_\Gamma\left(\psi+\psi_k\right)\mathrm{d}S-\lambda\int_\Gamma\mathcal{L}\left(\psi\right)\mathrm{d}S. \qquad (3.44)
\end{aligned}
$$

The growth assumptions (3.2)–(3.3) of the potentials f_0, g_0 together with the uniform V^1-estimate on (φ,ψ) from (3.43) yield that

$$
\begin{aligned}
\frac12\left|\int_\Omega\mu\mathrm{d}x\right|&\leqq\lambda\left|\int_\Omega\mu\mathrm{d}x\right|\\
&\leqq Q\left(\|(\varphi,\psi)\|_{V^1}\right)+\lambda\left|\Gamma\right|^{1/2}\left\|\mathcal{L}\left(\psi\right)\right\|_{L^2(\Gamma)}\\
&\leqq C_k, \qquad (3.45)
\end{aligned}
$$

for some positive function Q independent of λ, since $\lambda\leqq\sqrt{\lambda}$ when $\lambda\in[\frac12,1]$. Then for all $\lambda\in[0,1]$, using the above estimates for the mean value of the chemical potential μ and Poincaré's inequality, we can improve estimate (3.43) to

$$
\|\mathbf{v}\|_{\mathbb{H}^1(\Omega)}+\varepsilon^{1/q}\|\mathbf{v}\|_{\mathbb{W}^{1,q}(\Omega)}+\|\mu\|_{H^1(\Omega)}+\|(\varphi,\psi)\|_{V^1}\leqq C_k, \qquad (3.46)
$$

where C_k depends on h but is independent of λ.

Next, together with $(3.37)_1$, from the H^2-estimate (3.33) with

$$
\alpha:=-\lambda\frac{\varphi-\varphi_k}{h}-\lambda\mathbf{v}\cdot\nabla\varphi_k+\lambda\int_\Omega\mu\mathrm{d}x,
$$

we also get a uniform (in λ) estimate on the H^2-norm of the chemical potential μ such that

$$
\|\mu\|_{H^2}\leqq C_k. \qquad (3.47)
$$

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The same pointwise identities (see $(3.37)_2$ and $(3.37)_3$) allow us to write an elliptic boundary value problem for $(\varphi, \psi) \in V^2$ in the form

$$\begin{cases} -\Delta\varphi = h_1, & \text{in } \Omega, \\ -\Delta_{\boldsymbol{\tau}}\psi + \partial_{\mathbf{n}}\varphi + \zeta\psi = h_2, & \text{on } \Gamma, \end{cases} \tag{3.48}$$

where

$$h_1 = \lambda\mu + \lambda\frac{c_F}{2}(\varphi + \varphi_k) - \lambda f_0(\varphi) - \lambda\sigma\frac{\varphi - \varphi_k}{h},$$

$$h_2 = \lambda\mathcal{L}(\psi) + \lambda\frac{c_G}{2}(\psi + \psi_k) - \lambda g_0(\psi).$$

Owing to the estimate (3.46), we deduce from Lemma B.4 that

$$\|\varphi\|_{H^2} + \|\psi\|_{H^2(\Gamma)} \leqq C\left(\|h_1\|_{L^2} + \|h_2\|_{L^2(\Gamma)}\right) \leqq C_k. \tag{3.49}$$

Summing up, (3.45), (3.47) and (3.49) lead to the uniform (in λ) estimate

$$\|\mathbf{p}\|_X \leqq C_k,$$

where

$$\|\mathbf{p}\|_X = \left(\|\mathbf{v}\|_{\mathbb{H}^1} + \varepsilon^{1/q}\|\mathbf{v}\|_{\mathbb{W}^{1,q}}\right) + \|\mu\|_{H^2} + \|(\varphi, \psi)\|_{V^2}.$$

Finally, to get an estimate of $\mathcal{M}_k(\mathbf{p}) = \mathbf{f} \in \widetilde{Y}$, we recall that $\mathbf{f} = \lambda\mathcal{F}_k(\mathbf{p})$ (cf. (3.35)) and the fact that $\mathcal{F}_k : X \to \widetilde{Y}$ maps bounded sets into bounded sets, which holds due to the previous estimates for $\mathcal{F}_k$. As a consequence, we obtain

$$\|\mathbf{f}\|_{\widetilde{Y}} = \|\lambda\mathcal{F}_k(\mathbf{p})\|_{\widetilde{Y}} \leqq C_k(\|\mathbf{p}\|_X + 1) \leqq C_k,$$

which establishes the desired claim stated in (3.34).

Hence, the proof of Lemma 3.3 is complete. □

3.2. *Proof of Theorem 3.2*

Here we always assume that $\sigma, \varepsilon \in (0, 1]$.[1]

Step 1 (*Construction of approximating solutions*). Let $N \in \mathbb{N}$ be a given number and let $(\mathbf{v}_{k+1}, \mu_{k+1}, \varphi_{k+1}, \psi_{k+1})$ be chosen successively as a solution of the discrete problem (3.13)–(3.17) with $h = \frac{1}{N}$ and $(\mathbf{v}_0, \varphi_0^N, \psi_0^N)$ as the initial value. Here, the regularized initial datum $\left(\varphi_0^N, \psi_0^N\right) \in V^2$ is constructed in Lemma B.5 and it satisfies $\left(\varphi_0^N, \psi_0^N\right) \to (\varphi_0, \psi_0)$ in V^1 as $N \to \infty$. Furthermore, due to the convexity of the potentials F_0 and G_0, it follows that

$$F\left(\varphi_0^N\right) \to F(\varphi_0) \quad \text{in } L^1(\Omega),$$

$$G\left(\psi_0^N\right) \to G(\psi_0) \quad \text{in } L^1(\Gamma).$$

[1] Of course, bounds on $(\mathbf{v}, \mu, \varphi, \psi)$ depend explicitly on $\sigma, \varepsilon > 0$ in some places, but we choose not to show this dependence for the sake of the simplicity of notations.

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As in [5, Section 5], we define $f^N(t)$ on $[-h,\infty)$ through

$$f^N(t) = f_k \quad \text{for } t \in [(k-1)h, kh),$$

where $k \in \mathbb{N}_0$ and $f \in \{\mathbf{v}, \mu, \varphi, \psi\}$. In particular, it holds that

$$f^N((k-1)h) = f_k, \quad f^N(kh) = f_{k+1}, \quad \text{and } f^N(t) = f_{k+1} \quad \text{for } t \in [kh,(k+1)h).$$

Moreover, we define

$$f_h := f(t-h)$$

and

$$\left(\Delta_h^+ f\right)(t) := f(t+h) - f(t), \qquad \partial_{t,h}^+ f(t) := \frac{1}{h}\left(\Delta_h^+ f\right)(t),$$
$$\left(\Delta_h^- f\right)(t) := f(t) - f(t-h), \qquad \partial_{t,h}^- f(t) := \frac{1}{h}\left(\Delta_h^- f\right)(t).$$

We also set

$$\rho^N := \rho\left(\varphi^N\right).$$

Then, for arbitrary vector $\mathbf{w} \in C_0^\infty\left(0,T;\mathbb{C}_{\mathrm{div}}^\infty\left(\overline{\Omega}\right)\right)$, we shall choose $\widetilde{\mathbf{w}} := \int_{kh}^{(k+1)h} \mathbf{w}\mathrm{d}t$ as a test function in the weak formulation (3.13) and sum over $k \in \mathbb{N}_0$ to get

$$\begin{aligned}
&\int_0^T\int_\Omega \partial_{t,h}^-(\rho^N\mathbf{v}^N)\cdot\mathbf{w}\mathrm{d}x\mathrm{d}t + \int_0^T\int_\Omega \mathrm{div}\left(\rho_h^N\mathbf{v}^N\otimes\mathbf{v}^N\right)\cdot\mathbf{w}\mathrm{d}x\mathrm{d}t\\
&\quad + \varepsilon\int_0^T\int_\Omega\left(\left|D\mathbf{v}^N\right|^{q-2}D\mathbf{v}^N : D\mathbf{w} + \left|\mathbf{v}^N\right|^{q-2}\mathbf{v}^N\cdot\mathbf{w}\right)\mathrm{d}x\mathrm{d}t\\
&\quad + \int_0^T\int_\Omega 2\nu(\varphi_h^N)D\mathbf{v}^N : D\mathbf{w}\mathrm{d}x\mathrm{d}t + \int_0^T\int_\Gamma \beta(\psi_h^N)\mathbf{v}_{\boldsymbol{\tau}}^N\cdot\mathbf{w}_{\boldsymbol{\tau}}\mathrm{d}S\mathrm{d}t\\
&\quad - \int_0^T\int_\Omega\left(\mathbf{v}^N\otimes\mathbf{J}^N\right) : D\mathbf{w}\mathrm{d}x\mathrm{d}t\\
&= \int_0^T\int_\Omega \mu^N\nabla\varphi_h^N\cdot\mathbf{w}\mathrm{d}x\mathrm{d}t + \int_0^T\int_\Gamma \mathcal{L}\left(\psi^N\right)\nabla_{\boldsymbol{\tau}}\psi_h^N\cdot\mathbf{w}_{\boldsymbol{\tau}}\mathrm{d}S\mathrm{d}t\\
&\quad + \frac{1}{2}\int_0^T\int_\Omega R^N\mathbf{v}^N\cdot\mathbf{w}\mathrm{d}x\mathrm{d}t,
\end{aligned} \tag{3.50}$$

for all $\mathbf{w} \in C_0^\infty\left(0,T;\mathbb{C}_{\mathrm{div}}^\infty\left(\overline{\Omega}\right)\right)$, where by definition (see (3.12) and (3.19)) we have

$$\begin{cases} \mathbf{J}^N = -\rho'\left(\varphi_h^N\right)m(\varphi_h^N)\nabla\mu^N,\\ R^N = \partial_{t,h}^-\rho^N + \mathrm{div}\left(\rho_h^N\mathbf{v}^N + \mathbf{J}^N\right). \end{cases} \tag{3.51}$$

Using integration by parts, the first term in (3.50) can also be rewritten as

$$\int_0^T\int_\Omega \partial_{t,h}^-(\rho^N\mathbf{v}^N)\cdot\mathbf{w}\mathrm{d}x\mathrm{d}t = -\int_0^T\int_\Omega(\rho^N\mathbf{v}^N)\cdot\partial_{t,h}^+\mathbf{w}\mathrm{d}x\mathrm{d}t.$$

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Analogously, we deduce from (3.14)–(3.17) that

$$\int_0^T \int_\Omega \partial_{t,h}^- \varphi^N \xi \, \mathrm{d}x\mathrm{d}t - \int_0^T \int_\Omega \mathbf{v}^N \varphi_h^N \cdot \nabla \xi \, \mathrm{d}x\mathrm{d}t = - \int_0^T \int_\Omega m(\varphi_h^N) \nabla \mu^N \cdot \nabla \xi \, \mathrm{d}x\mathrm{d}t \tag{3.52}$$

for all $\xi \in C_0^\infty(0, T; H^1(\Omega))$, and

$$\int_0^T \int_\Gamma \partial_{t,h}^- \psi^N \theta \mathrm{d}S\mathrm{d}t + \int_0^T \int_\Gamma \left(\mathbf{v}_{\boldsymbol{\tau}}^N \cdot \nabla_{\boldsymbol{\tau}} \psi_h^N \right) \theta \mathrm{d}S\mathrm{d}t = - \int_0^T \int_\Gamma l_0 \left(\psi_h^N \right) \mathcal{L}(\psi^N) \theta \mathrm{d}S\mathrm{d}t \tag{3.53}$$

for all $\theta \in C_0^\infty(0, T; L^2(\Gamma))$, respectively. Furthermore, we have that the following equations:

$$\begin{cases} \mu^N + \dfrac{c_F}{2} \left(\varphi^N + \varphi_h^N \right) = -\Delta \varphi^N + f_0(\varphi^N) + \sigma \partial_{t,h}^- \varphi^N, \\ \mathcal{L}\left(\psi^N\right) + \dfrac{c_G}{2} \left(\psi^N + \psi_h^N \right) = -\Delta_{\boldsymbol{\tau}} \psi^N + \partial_{\mathbf{n}} \varphi^N + \zeta \psi^N + g_0\left(\psi^N\right), \end{cases} \tag{3.54}$$

which hold almost everywhere in Q_T and Σ_T, respectively.

Let now $E^N(t)$ be the piecewise linear interpolant of $E_{\mathrm{tot}}(\mathbf{v}_k, \varphi_k, \psi_k)$ at $t_k = kh$ given by

$$E^N(t) = \frac{(k+1)h - t}{h} E_{\mathrm{tot}}(\mathbf{v}_k, \varphi_k, \psi_k) + \frac{t - kh}{h} E_{\mathrm{tot}}(\mathbf{v}_{k+1}, \varphi_{k+1}, \psi_{k+1})$$

for $t \in [kh, (k+1)h)$. For all $t \in (kh, (k+1)h)$, $k \in \mathbb{N}_0$, we also define

$$\begin{aligned} \mathcal{D}^N(t) := & \int_\Omega 2\nu(\varphi_k) |D\mathbf{v}_{k+1}|^2 \mathrm{d}x + \int_\Gamma \beta(\psi_k) \left| (\mathbf{v}_{k+1})_{\boldsymbol{\tau}} \right|^2 \mathrm{d}S \\ & + \int_\Omega m(\varphi_k) |\nabla \mu_{k+1}|^2 \mathrm{d}x + \int_\Gamma l_0(\psi_k) |\mathcal{L}(\psi_{k+1})|^2 \mathrm{d}S \\ & + \varepsilon \int_\Omega \left(|D\mathbf{v}_{k+1}|^q + |\mathbf{v}_{k+1}|^q \right) \mathrm{d}x + \sigma \int_\Omega \left(\frac{\varphi_{k+1} - \varphi_k}{h} \right)^2 \mathrm{d}x. \end{aligned}$$

Then the discrete energy estimate obtained in Lemma 3.3 (cf. (3.21)) implies that

$$-\frac{\mathrm{d}}{\mathrm{d}t} E^N(t) = \frac{E_{\mathrm{tot}}(\mathbf{v}_k, \varphi_k, \psi_k) - E_{\mathrm{tot}}(\mathbf{v}_{k+1}, \varphi_{k+1}, \psi_{k+1})}{h} \geqq \mathcal{D}^N(t) \tag{3.55}$$

for all $t \in (t_k, t_{k+1})$, $k \in \mathbb{N}_0$.

Step 2 (*Passing to the limit as $N \to \infty$*). To complete the proof of Theorem 3.2, we shall pass to the limit as $h \to 0$ (resp. $N \to \infty$) in our approximating solutions.

Integrating (3.55) with respect to time gives

$$\begin{aligned} & E_{\mathrm{tot}}(\mathbf{v}^N(t), \varphi^N(t), \psi^N(t)) + \int_s^t \int_\Omega \left(2\nu(\varphi_h^N) |D\mathbf{v}^N|^2 + m(\varphi_h^N) |\nabla \mu^N|^2 \right) \mathrm{d}x\mathrm{d}\tau \\ & + \varepsilon \int_s^t \int_\Omega \left(|D\mathbf{v}^N|^q + |\mathbf{v}^N|^q \right) \mathrm{d}x\mathrm{d}\tau + \sigma \int_s^t \int_\Omega \left| \partial_{t,h}^- \varphi^N \right|^2 \mathrm{d}x\mathrm{d}\tau \end{aligned}$$

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$$+\int_s^t\int_\Gamma \left(\beta(\psi_h^N)|\mathbf{v}_{\boldsymbol{\tau}}^N|^2 + l_0(\psi_h^N)|\mathcal{L}\left(\psi^N\right)|^2\right) \mathrm{d}S\mathrm{d}\tau$$

$$\leqq E_{\mathrm{tot}}(\mathbf{v}^N(s), \varphi^N(s), \psi^N(s)) \tag{3.56}$$

for all $0 \leqq s \leqq t < T$ with $s, t \in h\mathbb{N}_0$.

Exploiting the fact that $E_{\mathrm{tot}}(\mathbf{v}_0, \varphi_0^N, \psi_0^N)$ is bounded (note that $F\left(\varphi_0^N\right) \in L^1(\Omega)$ and $G\left(\psi_0^N\right) \in L^1(\Gamma)$ hold uniformly in $N \to \infty$ in light of the assumptions), we infer from (3.56) the following uniform bounds:

$$\begin{cases} \mathbf{v}^N \text{ is bounded in } L^2(0,T;\mathbb{H}^1) \text{ and in } L^\infty(0,T;\mathbb{H}), \\ \nabla\mu^N \text{ is bounded in } L^2(0,T;\mathbb{L}^2(\Omega)), \\ \mathcal{L}\left(\psi^N\right) \text{ is bounded in } L^2(0,T;L^2(\Gamma)), \\ \left(\varphi^N,\psi^N\right) \text{ is bounded in } L^\infty(0,T;V^1), \\ F_0\left(\varphi^N\right) \text{ is bounded in } L^\infty(0,T;L^1(\Omega)), \\ G_0\left(\psi^N\right) \text{ is bounded in } L^\infty(0,T;L^1(\Gamma)), \\ \mathbf{J}^N \text{ is bounded in } L^2(0,T;\mathbb{L}^2(\Omega)), \\ \displaystyle\int_0^T \left|\int_\Omega \mu^N\,\mathrm{d}x\right| \mathrm{d}t \leqq \mathcal{Q}(T), \\ \sigma^{1/2}\partial_{t,h}^-\varphi^N \text{ is bounded in } L^2(0,T;L^2(\Omega)), \\ \varepsilon^{1/q}\mathbf{v}^N \text{ is bounded in } L^q\left(0,T;\mathbb{W}^{1,q}\right) \quad \text{for } q > 2d, \end{cases} \tag{3.57}$$

for a certain monotone function $\mathcal{Q} : \mathbb{R}^+ \to \mathbb{R}^+$. Moreover, we observe that

$$\begin{cases} f_0\left(\varphi^N\right) \text{ is bounded uniformly in } L^2\left(0,T;L^2(\Omega)\right), \\ g_0\left(\psi^N\right) \text{ is bounded uniformly in } L^2\left(0,T;L^2(\Gamma)\right), \end{cases} \tag{3.58}$$

due to the growth assumptions on f, g (see (3.3)), $(3.57)_4$ and the Sobolev embedding theorem.[2] Then by the elliptic estimate for problem (3.54) (recall Lemma B.4), (3.57) and (3.58), we can further derive that

$$\left(\varphi^N,\psi^N\right) \text{ is bounded uniformly in } L^2(0,T;V^2). \tag{3.59}$$

Using these bounds, we can pass to the limit for a subsequence (not relabelled for simplicity) to get the following preliminary convergent results:

$$\mathbf{v}^N \rightharpoonup \mathbf{v} \text{ in } L^2(0,T;\mathbb{H}^1), \tag{3.60}$$

$$\mathbf{v}^N \rightharpoonup^* \mathbf{v} \text{ in } L^\infty(0,T;\mathbb{H}) \cong \left(L^1(0,T;\mathbb{H})\right)^*, \tag{3.61}$$

$$\left(\varphi^N,\psi^N\right) \rightharpoonup^* (\varphi,\psi) \text{ in } L^\infty(0,T;V^1) \cong \left(L^1(0,T;(V^1)^*)\right)^*, \tag{3.62}$$

$$\left(\varphi^N,\psi^N\right) \rightharpoonup (\varphi,\psi) \text{ in } L^2(0,T;V^2), \tag{3.63}$$

[2] The bounds referred to here are indeed also uniform in (ε, σ).

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$$\mu^N \rightharpoonup \mu \ \text{ in } L^2(0,T;H^1(\Omega)), \tag{3.64}$$

$$\mathcal{L}\left(\psi^N\right) \rightharpoonup \mathcal{L}(\psi) \ \text{ in } L^2(0,T;L^2(\Gamma)), \tag{3.65}$$

$$\mathbf{J}^N \rightharpoonup \mathbf{J} \ \text{ in } L^2(0,T;\mathbb{L}^2(\Omega)), \tag{3.66}$$

$$\sigma^{\frac{1}{2}}\partial_{t,h}^{-}\varphi^N \rightharpoonup \sigma^{\frac{1}{2}}\partial_t\varphi \ \text{ in } L^2(0,T;L^2(\Omega)), \tag{3.67}$$

$$\varepsilon^{1/q}\mathbf{v}^N \rightharpoonup \varepsilon^{1/q}\mathbf{v} \ \text{ in } L^q\left(0,T;\mathbb{W}^{1,q}\right). \tag{3.68}$$

Remark 3.6. Here and after, all limits must be understood for suitable convergent subsequences $N_k \to \infty$ (resp. $h_k \to 0$) for $k \to \infty$, unless otherwise stated. We also use the abbreviation "$\in_\sigma$" to mean that the corresponding bounds are independent of N in the associated spaces, but will blow up as $\sigma \to 0^+$.

Next, let $\widetilde{\varphi}^N$ be the piecewise linear interpolant of $\varphi^N(t_k)$, where $t_k = kh$, $k \in \mathbb{N}_0$, namely, $\widetilde{\varphi}^N = \frac{1}{h}\chi_{[0,h]} *_t \varphi^N$, where the convolution is only taken with respect to the time variable t. By a similar construction, we also define $\widetilde{\psi}^N$ such that $\widetilde{\psi}^N = \frac{1}{h}\chi_{[0,h]} *_t \psi^N$. Then it follows that

$$\partial_t\widetilde{\varphi}^N = \partial_{t,h}^{-}\varphi^N, \quad \partial_t\widetilde{\psi}^N = \partial_{t,h}^{-}\psi^N$$

and

$$\|\widetilde{\varphi}^N - \varphi^N\|_{(H^1(\Omega))^*} \leqq h\|\partial_t\widetilde{\varphi}^N\|_{(H^1(\Omega))^*}, \quad \|\widetilde{\psi}^N - \psi^N\|_{L^2(\Gamma)} \leqq h\|\partial_t\widetilde{\psi}^N\|_{L^2(\Gamma)}. \tag{3.69}$$

From equation (3.52) and the estimates $(3.57)_1$, $(3.57)_2$ and $(3.57)_4$, we obtain that

$$\partial_t\widetilde{\varphi}^N \in L^2(0,T;(H^1(\Omega))^*)$$

is bounded, since $\mathbf{v}^N\varphi_h^N$ and $\nabla\mu^N$ are both bounded in $L^2(0,T;\mathbb{L}^2(\Omega))$. On the other hand, from $(3.57)_1$, $(3.57)_3$, $(3.57)_4$ together with (3.59), we see that $l_0\left(\psi^N\right)\mathcal{L}(\psi^N)$ is bounded in $L^2\left(0,T;L^2(\Gamma)\right)$ and moreover, $\mathbf{v}_{\tau_j}^N\partial_{\tau_j}\psi^N$ is bounded in $L^{4/3}\left(0,T;L^2(\Gamma)\right)$ if $d=3$ and in $L^{\frac{4s}{3s-2}}\left(0,T;L^2(\Gamma)\right)$ for $s\in(2,\infty)$, if $d=2$. As a result, it follows from equation (3.53) that

$$\partial_t\widetilde{\psi}^N \text{ is uniformly bounded in } \begin{cases} L^{4/3}\left(0,T;L^2(\Gamma)\right), & \text{if } d=3,\\ L^{\frac{4s}{3s-2}}\left(0,T;L^2(\Gamma)\right), & \text{if } d=2,\ s>2. \end{cases} \tag{3.70}$$

We remark that (3.70) can also be improved to $\partial_t\widetilde{\psi}^N \in L^2(0,T;L^2(\Gamma))$ using the last estimate in (3.57). Together with the boundedness of $(\widetilde{\varphi}^N,\widetilde{\psi}^N)$ in $L^\infty(0,T;V^1)$, which follows from the estimates of $\left(\varphi^N,\psi^N\right)$ in $L^\infty(0,T;V^1)$, we get, with the help of the lemma of Aubin–Lions–Simon (see Lemma B.1), the strong convergence

$$(\widetilde{\varphi}^N,\widetilde{\psi}^N) \to (\widetilde{\varphi},\widetilde{\psi}) \ \text{ in } C([0,T];V^{1-s}), \quad \forall s\in\left(0,\frac{1}{2}\right) \tag{3.71}$$

for some

$$(\widetilde{\varphi},\widetilde{\psi}) \in L^\infty(0,T;V^1).$$

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In particular, it holds for a subsequence that

$$(\widetilde{\varphi}^N, \widetilde{\psi}^N) \to (\widetilde{\varphi}, \widetilde{\psi}) \quad \text{almost everywhere in} \quad \overline{\Omega} \times (0, T).$$

On the other hand, we infer from (3.69) that

$$\begin{cases} \widetilde{\varphi}^N - \varphi^N \to 0 & \text{in } L^2(0, T; (H^1(\Omega))^*), \\ \widetilde{\psi}^N - \psi^N \to 0 & \text{in } L^{4/3}(0, T; L^2(\Gamma)), \end{cases} \tag{3.72}$$

which yields

$$\widetilde{\varphi} = \varphi \quad \text{and} \quad \widetilde{\psi} = \psi.$$

Furthermore, since

$$\widetilde{\varphi}^N \in H^1(0, T; (H^1(\Omega))^*) \cap L^2(0, T; H^2(\Omega)) \hookrightarrow C([0, T]; H^{1-s}(\Omega)),$$
$$\widetilde{\psi}^N = \mathrm{tr}\left(\widetilde{\varphi}^N\right) \in W^{1,4/3}(0, T; L^2(\Gamma)) \cap L^2(0, T; H^2(\Gamma)) \hookrightarrow C([0, T]; H^{1-s}(\Gamma))$$

for some $s \in (1/2, 1)$ as well as $(\widetilde{\varphi}^N, \widetilde{\psi}^N) \in L^\infty(0, T; V^1)$ is bounded, it also follows that

$$(\varphi, \psi) = (\widetilde{\varphi}, \widetilde{\psi}) \in C_w([0, T]; V^1).$$

To verify the initial condition $(\varphi(0), \psi(0)) = (\varphi_0, \psi_0)$, we first observe that

$$\widetilde{\varphi}^N(0) \rightharpoonup^* \widetilde{\varphi}(0) = \varphi(0), \qquad \text{in } (H^1(\Omega))^*,$$
$$\widetilde{\psi}^N(0) = \mathrm{tr}\widetilde{\varphi}^N(0) \rightharpoonup^* \widetilde{\psi}(0) = \psi(0), \qquad \text{in } L^2(\Gamma).$$

Furthermore, it holds that $\widetilde{\varphi}^N(0) = \varphi_0^N$ and $\widetilde{\psi}^N(0) = \psi_0^N$, with the right-hand sides converging strongly to φ_0 in $L^2(\Omega)$ and to ψ_0 in $L^2(\Gamma)$, respectively. Then we can conclude that

$$\varphi(0) = \varphi_0 \quad \text{and} \quad \psi(0) = \psi_0.$$

The estimates (3.71) and (3.72) yield the strong convergence results

$$\begin{cases} \varphi^N - \varphi \to 0 & \text{in } L^2(0, T; (H^1(\Omega))^*), \\ \psi^N - \psi \to 0 & \text{in } L^{4/3}(0, T; L^2(\Gamma)), \end{cases} \tag{3.73}$$

which together with (3.59), (3.63) and suitable interpolation inequalities further imply that

$$\begin{cases} \varphi^N \to \varphi & \text{in } L^2(0, T; H^{2-s}(\Omega)), \\ \psi^N \to \psi & \text{in } L^{\frac{8}{6-s}}(0, T; H^{2-s}(\Gamma)) \end{cases} \tag{3.74}$$

for $s \in (0, 2)$. Then we have the pointwise convergence $(\varphi^N, \psi^N) \to (\varphi, \psi)$ almost everywhere in $\overline{\Omega} \times (0, T)$. Combining this fact with the continuity of f_0, g_0 and (3.58), we can deduce the (weak) convergence for the nonlinear terms $f_0 = F_0'$, $g_0 = G_0'$, namely,

$$\begin{cases} f_0\left(\varphi^N\right) \rightharpoonup f_0(\varphi) & \text{in } L^2(0, T; L^2(\Omega)), \\ g_0\left(\psi^N\right) \rightharpoonup g_0(\psi) & \text{in } L^2(0, T; L^2(\Gamma)), \end{cases} \tag{3.75}$$

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owing to the Lebesgue convergence theorem (see Lemma B.2). Concerning the nonlinear density function ρ, due to the boundedness of ρ', ρ'', we infer from (3.74) and the pointwise convergence of φ^N that

$$\rho(\varphi^N) \to \rho(\varphi) \quad \text{in } L^2(0,T;H^1(\Omega)) \cap L^p(Q_T), \quad \forall\, p \in [2,\infty). \tag{3.76}$$

In a similar manner, for $p \in [2,\infty)$, we have

$$\begin{aligned} m(\varphi^N) &\to m(\varphi), \quad \nu(\varphi^N) \to \nu(\varphi) \quad \text{in } L^p(Q_T),\\ l_0(\psi^N) &\to l_0(\psi), \quad \beta(\psi^N) \to \beta(\psi) \quad \text{in } L^p(\Sigma_T). \end{aligned}$$

It easily follows the above facts and (3.51), (3.64) and (3.66) that the weak limit of $\mathbf{J}^N$ can be identified as

$$\mathbf{J} = -\rho'(\varphi)m(\varphi)\nabla\mu \quad \text{in } L^2(0,T;\mathbb{L}^2(\Omega)).$$

Next, taking advantage of (3.63), (3.67), (3.75), and the fact that the left-hand sides of (3.54) converge to $\mu + c_F\varphi + \sigma\partial_t\varphi$ and $\mathcal{L}(\psi) + c_G\psi$, respectively as $N \to \infty$ up to a subsequence (in light of the properties (3.64) and (3.65)), we finally deduce that

$$\begin{cases} \mu + c_F\varphi = -\Delta\varphi + f_0(\varphi) + \sigma\partial_t\varphi, & \text{in } L^2(0,T;L^2(\Omega)),\\ \mathcal{L}(\psi) + c_G\psi = -\Delta_{\boldsymbol{\tau}}\psi + \partial_{\mathbf{n}}\varphi + \zeta\psi + g_0(\psi), & \text{in } L^2(0,T;L^2(\Gamma)). \end{cases} \tag{3.77}$$

In (3.77), we also note that $f_0(r) - c_F r = f(r)$ and $g_0(r) - c_G r = g(r)$. Taking $s \in (0,1/2)$ in (3.74), it also holds that

$$\left(\varphi^N,\psi^N\right) \to (\varphi,\psi) \text{ in } L^{\frac{8}{6-s}}\left(0,T;V^{2-s}\right) \hookrightarrow L^{\frac{8}{6-s}}\left(0,T;L^\infty(\Omega)\times L^\infty(\Gamma)\right), \tag{3.78}$$

with strong convergence.

Our next aim is to show the strong convergence $\mathbf{v}^N \to \mathbf{v}$ in $L^2(0,T;\mathbb{H})$. First, owing to the fact for $\rho_h^N = \rho(\varphi_h^N)$ that

$$\rho\left(\varphi_h^N\right),\ \rho'(\varphi_h^N) \in L^\infty(Q_T)$$

are bounded by Assumption 2, and using suitable interpolation inequalities, we can obtain the following bounds (cf. [5, Section 5, (i)–(iv), pp. 474]):

$$\begin{cases} \rho_h^N\mathbf{v}^N\otimes\mathbf{v}^N & \text{is bounded in } L^2(0,T;L^{3/2}(\Omega)^{d\times d}),\\ D\mathbf{v}^N & \text{is bounded in } L^2(0,T;\mathbb{L}^2(\Omega)),\\ \mathbf{v}^N\otimes\nabla\mu^N & \text{is bounded in } L^{8/7}(0,T;L^{4/3}(\Omega)^{d\times d}),\\ \mu^N\nabla\varphi_h^N & \text{is bounded in } L^2(0,T;\mathbb{L}^{3/2}(\Omega)). \end{cases} \tag{3.79}$$

Then we see that that all the four terms in (3.79) are bounded in $L^{8/7}(0,T;L^{4/3}(\Omega))$, in particular, the third estimate also implies that

$$\mathbf{v}^N\otimes\mathbf{J}^N \quad \text{is bounded in } L^{8/7}(0,T;L^{4/3}(\Omega)^{d\times d}).$$

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In addition, exploiting the interpolation inequality

$$\|\psi\|_{W^{1,8/3}(\Gamma)} \leqq C \|\psi\|_{H^2(\Gamma)}^{1/4} \|\psi\|_{H^1(\Gamma)}^{3/4}$$

with the third and fourth estimates in (3.57) and (3.59), we have

$$\begin{aligned}
&\left\| \left(\mathcal{L}\left(\psi^N\right) \nabla_{\boldsymbol{\tau}} \psi_h^N, \mathbf{w}_{\boldsymbol{\tau}} \right)_\Gamma \right\|_{L^{4/3}(0,T)} \\
&\quad \leqq C \|\mathcal{L}\left(\psi^N\right)\|_{L^2(0,T;L^2(\Gamma))} \|\psi\|_{L^2(0,T;H^2(\Gamma))}^{1/4} \|\psi\|_{L^\infty(0,T;H^1(\Gamma))}^{3/4} \|\mathbf{w}_{\boldsymbol{\tau}}\|_{L^8(0,T;\mathbb{L}^8(\Gamma))} \\
&\quad \leqq C \|\mathbf{w}_{\boldsymbol{\tau}}\|_{L^8(0,T;\mathbb{L}^8(\Gamma))}, \quad \forall\, \mathbf{w}_{\boldsymbol{\tau}} \in L^8(0,T;\mathbb{L}^8(\Gamma)).
\end{aligned} \tag{3.80}$$

Therefore, it follows that

$$\sup_{\|\mathbf{w}\|_{L^8(0,T;\mathbb{W}^{1,4})} \leqq 1} \left| \left(\mathcal{L}\left(\psi^N\right) \nabla_{\boldsymbol{\tau}} \psi_h^N, \mathbf{w}_{\boldsymbol{\tau}} \right)_\Gamma \right| \text{ is bounded in } L^{4/3}(0,T) \subset L^{8/7}(0,T), \tag{3.81}$$

since for $\mathbf{w} \in \overline{\mathbb{C}_{\mathrm{div}}^\infty\left(\overline{\Omega}\right)}^{\mathbb{W}^{1,4}} := \mathbb{W}_{\mathrm{div}}^{1,4} \subset \mathbb{W}^{1,4}(\Omega)$ it holds that $\mathrm{tr}(\mathbf{w}) \in \mathbb{W}^{3/4,4}(\Gamma) \hookrightarrow \mathbb{L}^8(\Gamma)$, and so does its tangential component $\mathbf{w}_{\boldsymbol{\tau}}$. In view of the equation (3.50), it remains to estimate the last term $R^N \mathbf{v}^N$. This requires some improved estimates for the case $\sigma > 0$ and relies on the definition of R^N in (3.51). For each $\sigma > 0$, we have, from (3.67) that $\partial_{t,h}^- \varphi^N \in_\sigma L^2\left(0,T;L^2(\Omega)\right)$ is bounded. Then thanks to the boundedness of ρ', ρ'' and (3.74), we have, for any $\eta \in C(Q_T)$,

$$\begin{aligned}
&\left| \int_0^T\!\!\int_\Omega \left(\partial_{t,h}^- \rho(\varphi^N) - \rho'(\varphi)\partial_t \varphi \right) \eta \,\mathrm{d}x\,\mathrm{d}t \right| \\
&\quad \leqq \left| \int_0^T\!\!\int_\Omega \left(\partial_{t,h}^- \rho(\varphi^N) - \rho'(\varphi^N)\partial_{t,h}^- \varphi^N \right) \eta \,\mathrm{d}x\,\mathrm{d}t \right| \\
&\qquad + \left| \int_0^T\!\!\int_\Omega \left(\rho'(\varphi^N)\partial_{t,h}^- \varphi^N - \rho'(\varphi)\partial_{t,h}^- \varphi^N \right) \eta \,\mathrm{d}x\,\mathrm{d}t \right| \\
&\qquad + \left| \int_0^T\!\!\int_\Omega \rho'(\varphi)\left(\partial_{t,h}^- \varphi^N - \partial_t \varphi \right) \eta \,\mathrm{d}x\,\mathrm{d}t \right| \\
&\quad \leqq \|\rho''\|_{L^\infty(Q_T)} \|\partial_{t,h}^- \varphi^N\|_{L^2(0,T;L^2(\Omega))}^2 \|\eta\|_{L^\infty(Q_T)} h \\
&\qquad + \|\rho''\|_{L^\infty(Q_T)} \|\varphi^N - \varphi\|_{L^2(0,T,L^\infty(\Omega))} \|\partial_{t,h}^- \varphi^N\|_{L^2(0,T;L^2(\Omega))} \|\eta\|_{L^\infty(0,T;L^2(\Omega))} \\
&\qquad + \left| \int_0^T\!\!\int_\Omega \left(\partial_{t,h}^- \varphi^N - \partial_t \varphi \right) \left(\rho'(\varphi)\eta \right) \mathrm{d}x\,\mathrm{d}t \right| \\
&\quad \to 0,
\end{aligned}$$

as $N \to \infty$ (up to a subsequence), which implies the sequential convergence

$$\partial_{t,h}^- \rho(\varphi^N) \to \rho'(\varphi)\partial_t \varphi$$

in the sense of distribution. Next, we find from (3.51) that

$$\left\langle R^N \mathbf{v}^N, \mathbf{w} \right\rangle = \left(\partial_{t,h}^- \rho^N \mathbf{v}^N, \mathbf{w} \right)_\Omega - \left(\rho_h^N \mathbf{v}^N + \mathbf{J}^N, \nabla\left(\mathbf{v}^N \cdot \mathbf{w} \right) \right)_\Omega \tag{3.82}$$

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for any smooth test function $\mathbf{w} \in \mathbb{C}^{\infty}_{\mathrm{div}}(\overline{\Omega})$. Since $\mathbf{v}_i^N \mathbf{w}_i$ is bounded in $H^1(\Omega)$ as a product of functions in $H^1(\Omega) \times H^{3/2+\delta}(\Omega)$, for some $\delta > 0$ (cf. Lemma B.3), we infer from (3.82), the seventh and ninth estimates in (3.57) on $\mathbf{J}^N$ and $\partial^-_{t,h}\rho(\varphi^N)$ that

$$\sup_{\|\mathbf{w}\|_{L^\infty(0,T;\mathbb{H}^{3/2+\delta})} \leqq 1} \left|\left\langle R^N \mathbf{v}^N, \mathbf{w}\right\rangle\right| \in_\sigma L^1(0,T), \tag{3.83}$$

because $\nabla\left(\mathbf{v}_i^N \mathbf{w}_i\right) \in L^2(0,T;\mathbb{L}^2(\Omega))$ is bounded, for any $\mathbf{w} \in L^\infty\left(0,T;\mathbb{H}^{3/2+\delta}\right)$ with $\delta > 0$. Therefore, on account of (3.79), (3.81) and (3.83), we can allow in the weak formulation (3.50) for test functions with $\mathbf{w} \in L^\infty(0,T;\mathbb{H}^{3/2+\delta}) \hookrightarrow L^8(0,T;\mathbb{W}^{1,4}(\Omega))$, provided that $\delta \geqq 1/4$.

Now let $\widetilde{\rho\mathbf{v}}^N$ be the piecewise linear interpolant of $\left(\rho^N \mathbf{v}^N\right)(t_k)$, where $t_k = kh$, $k \in \mathbb{N}_0$. By definition, it holds that

$$\partial_t(\widetilde{\rho\mathbf{v}}^N) = \partial^-_{t,h}\left(\rho^N \mathbf{v}^N\right).$$

Hence, from the equation (3.50), the last estimate in (3.57) and estimates (3.79), (3.81) and (3.83), we obtain

$$\begin{aligned}\partial_t(\mathbb{P}(\widetilde{\rho\mathbf{v}}^N)) &\in \left(L^\infty(0,T;\mathbb{H}^{3/2+\delta}) \oplus L^q\left(0,T;\mathbb{W}^{1,q}(\Omega)\right)\right)^* \\ &= L^1(0,T;\mathbb{H}^{-3/2-\delta}) \oplus L^{\frac{q}{q-1}}\left(0,T;\left(\mathbb{W}^{1,q}(\Omega)\right)^*\right)\end{aligned}$$

for any $\delta \geqq 1/4$, $q > 2d$, where $\mathbb{P}$ is the Helmholtz–Leray projection $\mathbb{P} : L^2(0,T;\mathbb{L}^2(\Omega)) \to L^2(0,T;\mathbb{H})$. Noting that $\mathbb{P}(\widetilde{\rho\mathbf{v}}^N) \in L^2(0,T;\mathbb{W}^{1,2}(\Omega))$ is bounded, then we can therefore conclude from Lemma B.1 the strong convergence

$$\mathbb{P}(\widetilde{\rho\mathbf{v}}^N) \to \mathbf{v}^* \quad \text{in } L^2(0,T;\mathbb{H}) \tag{3.84}$$

for some vectorial function $\mathbf{v}^* \in L^\infty(0,T;\mathbb{H})$. We also infer the following weak convergence results from (3.60), (3.76) and the boundedness of ρ:

$$(\rho^N)^\gamma \mathbf{v}^N \rightharpoonup \rho^\gamma \mathbf{v} \quad \text{in } L^2(0,T;\mathbb{L}^2(\Omega)), \quad \text{for } \gamma = 1, \frac{1}{2}. \tag{3.85}$$

Observing that

$$\|\mathbb{P}(\widetilde{\rho\mathbf{v}}^N) - \mathbb{P}(\rho^N\mathbf{v}^N)\|_{L^{8/7}(0,T;(\mathbb{W}^{1,4})^*)} \leqq h\|\partial_t(\mathbb{P}(\widetilde{\rho\mathbf{v}}^N))\|_{L^{8/7}(0,T;(\mathbb{W}^{1,4})^*)} \to 0$$

as $h \to 0$, since the projection $\mathbb{P}$ is weakly continuous, then it follows from (3.84) and (3.85) with $\gamma = 1$ that

$$\mathbf{v}^* = \mathbb{P}(\rho\mathbf{v}).$$

Moreover, since $\mathbb{P}(\rho^N\mathbf{v}^N) \in L^2(0,T;\mathbb{W}^{1,2}(\Omega)) \cap L^\infty(0,T;\mathbb{L}^2(\Omega))$, from the above strong convergence result and interpolation inequality, we have

$$\mathbb{P}(\rho^N\mathbf{v}^N) \to \mathbb{P}(\rho\mathbf{v}) \quad \text{in } L^2(0,T;\mathbb{H}).$$

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This fact and the weak convergence of $\mathbf{v}^N$ in $L^2(0,T;\mathbb{H})$ entail that

$$\begin{aligned}\int_0^T\int_\Omega \rho^N|\mathbf{v}^N|^2 \mathrm{d}x\mathrm{d}t &= \int_0^T\int_\Omega \mathbb{P}(\rho^N\mathbf{v}^N)\cdot\mathbf{v}^N \mathrm{d}x\mathrm{d}t\\ &\longrightarrow \int_0^T\int_\Omega \mathbb{P}(\rho\mathbf{v})\cdot\mathbf{v}\mathrm{d}x\mathrm{d}t\\ &= \int_0^T\int_\Omega \rho\,|\mathbf{v}|^2\mathrm{d}x\mathrm{d}t,\end{aligned}$$

which together with (3.85) (taking $\gamma = 1/2$) further yields the strong convergence

$$(\rho^N)^{1/2}\mathbf{v}^N \to \rho^{1/2}\mathbf{v} \quad \text{in} \quad L^2(0,T;\mathbb{L}^2(\Omega)).$$

By (3.76), we also have $\rho(\varphi^N)\to\rho(\varphi)$ almost everywhere in Q_T. Hence, we can conclude from the above fact and $\rho^N \geqq \rho_0 > 0$ that

$$\mathbf{v}^N = (\rho^N)^{-1/2}\left((\rho^N)^{1/2}\mathbf{v}^N\right) \to \mathbf{v} \ \text{ in } \ L^2(0,T;\mathbb{L}^2(\Omega)). \tag{3.86}$$

Recalling the first estimate in (3.57) and using interpolation, we also have

$$\mathbf{v}^N \to \mathbf{v} \ \text{ in } \ L^2(0,T;\mathbb{H}^{1-s}(\Omega)), \quad s\in(0,1]. \tag{3.87}$$

Then it follows that (for a proper subsequence)

$$\mathbf{v}^N \to \mathbf{v} \quad \text{almost everywhere in} \quad Q_T.$$

Moreover, one can also show that the velocity $\mathbf{v}$ fulfills the initial condition $\mathbf{v}(0) = \mathbf{v}_0$ in $\mathbb{L}^2(\Omega)$ thanks to Lemma B.7 and arguing as in [5, Section 5.2].

Finally, we can pass to the limit as $N\to\infty$ (up to a subsequence) in (3.50)–(3.54) to show that the limit $(\mathbf{v},\mu,\varphi,\psi)$ is indeed a weak solution in the sense of Definition 3.1 for each fixed $\sigma,\varepsilon>0$.

Owing to the strong convergence

$$\left(\varphi^N,\psi^N\right)\longrightarrow(\varphi,\psi) \quad \text{in } L^4\left(0,T;V^1\right),$$

which follows by interpolation using (3.74) and the boundedness of $\left(\varphi^N,\psi^N\right)\in L^\infty(0,T;V^1)$, the passage to the limit on the right-hand side of (3.50) is reasonably straightforward. Indeed, since $\mu^N \rightharpoonup \mu$ in $L^2\left(0,T;H^1(\Omega)\right)$ and $\mathcal{L}\left(\psi^N\right)\rightharpoonup\mathcal{L}(\psi)$ in $L^2(0,T;L^2(\Gamma))$, we get

$$\begin{aligned}\int_0^T\int_\Omega \mu^N\nabla\varphi_h^N\cdot\mathbf{w}\mathrm{d}x\mathrm{d}t &= -\int_0^T\int_\Omega \left(\nabla\mu^N\varphi_h^N\right)\cdot\mathbf{w}\mathrm{d}x\mathrm{d}t\\ &\longrightarrow -\int_0^T\int_\Omega (\nabla\mu\varphi)\cdot\mathbf{w}\mathrm{d}x\mathrm{d}t\\ &= \int_0^T\int_\Omega \mu\nabla\varphi\cdot\mathbf{w}\mathrm{d}x\mathrm{d}t \end{aligned}\tag{3.88}$$

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and

$$\int_0^T \int_\Gamma \mathcal{L}\left(\psi^N\right) \nabla_{\boldsymbol{\tau}} \psi_h^N \cdot \mathbf{w}_\tau \mathrm{d}S\mathrm{d}t \longrightarrow \int_0^T \int_\Gamma \mathcal{L}(\psi) \nabla_{\boldsymbol{\tau}} \psi \cdot \mathbf{w}_{\boldsymbol{\tau}} \mathrm{d}S\mathrm{d}t \tag{3.89}$$

for all divergence free $\mathbf{w} \in C_0^\infty(0, T; \mathbb{H}^{3/2+\delta} \cap \mathbb{W}^{1,q}(\Omega))$, where $\delta \geqq 1/4$ and $q > 2d$. Next, by (3.61) and (3.87) we have the strong convergence

$$\mathbf{v}^N \longrightarrow \mathbf{v} \quad \text{in } L^p(0, T; \mathbb{L}^4(\Omega)) \text{ for any } p \in [1, 8/3),$$

from which we infer that

$$\mathbf{v}_i^N \mathbf{v}_j^N \longrightarrow \mathbf{v}_i \mathbf{v}_j \quad \text{in } L^l(0, T; L^2(\Omega)) \text{ for any } l \in [1, 4/3).$$

Due to (3.68) and (3.87), we also have the strong convergence

$$D\mathbf{v}^N \longrightarrow D\mathbf{v} \quad \text{in } L^2(0, T; L^4(\Omega)^{d\times d}), \tag{3.90}$$

which improves upon (3.87) when $\varepsilon > 0$. Then we can deduce that, for all $\mathbf{w} \in C_0^\infty(0, T; \mathbb{H}^{3/2+\delta} \cap \mathbb{W}^{1,q}(\Omega))$ (with $\delta \geqq 1/4$), it holds that

$$\left\langle R^N \mathbf{v}^N, \mathbf{w} \right\rangle \to \langle R_\sigma \mathbf{v}, \mathbf{w} \rangle,$$

where

$$\langle R_\sigma \mathbf{v}, \mathbf{w} \rangle := \left((\rho'(\varphi)\,\partial_t \varphi)\mathbf{v}, \mathbf{w}\right)_{Q_T} - \left((\rho\mathbf{v} + \mathbf{J}), \nabla(\mathbf{v}\cdot\mathbf{w})\right)_{Q_T}. \tag{3.91}$$

Passing to the limit in (3.52)–(3.54) to recover (3.5)–(3.8) is also straightforward on account of (3.62)–(3.67), (3.70), (3.74) and (3.75).

In summary, we obtain that

$$\begin{aligned}
&-(\rho\mathbf{v}, \partial_t \mathbf{w})_{Q_T} + (\operatorname{div}(\rho\mathbf{v}\otimes\mathbf{v}), \mathbf{w})_{Q_T} + (2\nu(\varphi)D\mathbf{v}, D\mathbf{w})_{Q_T} \\
&\quad + (\beta(\psi)\mathbf{v}_{\boldsymbol{\tau}}, \mathbf{w}_{\boldsymbol{\tau}})_{\Sigma_T} + \varepsilon\left(|D\mathbf{v}|^{q-2} D\mathbf{v}, D\mathbf{w}\right)_{Q_T} + \varepsilon\left(|\mathbf{v}|^{q-2}\mathbf{v}, \mathbf{w}\right)_{Q_T} \\
&= ((\mathbf{v}\otimes\mathbf{J}), D\mathbf{w})_{Q_T} + \frac{1}{2}\langle R_\sigma, \mathbf{w}\rangle + (\mu\nabla\varphi, \mathbf{w})_{Q_T} \\
&\quad + (\mathcal{L}(\psi)\nabla_{\boldsymbol{\tau}}\psi, \mathbf{w}_{\boldsymbol{\tau}})_{\Sigma_T}
\end{aligned} \tag{3.92}$$

for all $\mathbf{w} \in C_0^\infty(0, T; \mathbb{H}^{3/2+\delta} \cap \mathbb{W}^{1,q}(\Omega))$, as well as

$$-(\varphi, \partial_t \xi)_{Q_T} + (\mathbf{v}\cdot\nabla\varphi, \xi)_{Q_T} = -(m(\varphi)\nabla\mu, \nabla\xi)_{Q_T} \tag{3.93}$$

for all $\xi \in C_0^\infty(0, T; H^1(\Omega))$.

Observe now that (3.93) can be written in a stronger form, namely,

$$\left\langle \partial_t\varphi, \tilde{\xi}\right\rangle + \left(\mathbf{v}\cdot\nabla\varphi, \tilde{\xi}\right)_\Omega = -\left(m(\varphi)\nabla\mu, \nabla\tilde{\xi}\right)_\Omega \tag{3.94}$$

for all $\tilde{\xi} \in H^1(\Omega)$ and almost everywhere in $[0, T]$. Hence, choosing

$$\tilde{\xi} = \rho'(\varphi(t))\,\mathbf{v}(t)\cdot\mathbf{w}(t)$$

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in (3.94) and recalling (1.16) and (3.91), we deduce that

$$\langle R_\sigma \mathbf{v}, \mathbf{w}\rangle = -\int_{Q_T} m(\varphi)\left(\nabla \rho'(\varphi)\cdot\nabla\mu\right)\mathbf{v}\cdot\mathbf{w}\,\mathrm{d}x\,\mathrm{d}t = \langle R\mathbf{v}, \mathbf{w}\rangle \tag{3.95}$$

for all $\mathbf{w} \in C_0^\infty(0, T; \mathbb{H}^{3/2+\delta} \cap \mathbb{W}^{1,q}(\Omega))$.

Step 3 (*Dissipative energy inequality*). Multiplying the discrete energy inequality (3.55) by $\eta \in W^{1,1}(0, T)$ with $\eta \geqq 0$, $\eta(T) = 0$ and using integration by parts, we obtain

$$E_{\mathrm{tot}}(\mathbf{v}_0, \varphi_0^N, \psi_0^N)\eta(0) + \int_0^T E^N(t)\eta'(t)\mathrm{d}t \geqq \int_0^T \mathcal{D}^N(t)\eta(t)\mathrm{d}t. \tag{3.96}$$

Because of the strong convergence of $\mathbf{v}^N$ and $\left(\varphi^N, \psi^N\right)$ (recall (3.74) and (3.86)), we have

$$\mathbf{v}^N(t) \to \mathbf{v}(t) \quad \text{in } \mathbb{H},$$
$$\left(\varphi^N(t), \psi^N(t)\right) \to (\varphi(t), \psi(t)) \quad \text{in } C(\overline{\Omega}) \times C(\Gamma)$$

for almost every $t \in (0, T)$, along a proper subsequence. Then it holds that

$$E^N(t) \to E_{\mathrm{tot}}(\mathbf{v}(t), \varphi(t), \psi(t)) \ \text{ for almost all } \ t \in (0, T).$$

Moreover, by the lower semicontinuity of norms and the almost everywhere convergence of $\left(\varphi^N, \psi^N\right)$ to (φ, ψ), the inequality

$$\liminf_{N\to\infty} \int_0^T \mathcal{D}^N(t)\eta(t)\mathrm{d}t \geqq \int_0^T \mathcal{D}(t)\eta(t)\mathrm{d}t$$

for all $\eta \in W^{1,1}(0, T)$ with $\eta \geqq 0$ holds, where

$$\mathcal{D}(t) := \int_\Omega 2\nu(\varphi)|D\mathbf{v}|^2\mathrm{d}x + \int_\Gamma \beta(\psi)\,|\mathbf{v}_{\boldsymbol{\tau}}|^2\,\mathrm{d}S + \int_\Omega m(\varphi)|\nabla\mu|^2\mathrm{d}x$$
$$+ \int_\Gamma l_0(\psi)\,|\mathcal{L}(\psi)|^2\,\mathrm{d}S + \varepsilon\int_\Omega \left(|D\mathbf{v}|^q + |\mathbf{v}|^q\right)\mathrm{d}x + \sigma\int_\Omega |\partial_t\varphi|^2\,\mathrm{d}x.$$

Hence, passing to the limit in (3.96), we obtain

$$E_{\mathrm{tot}}(\mathbf{v}_0, \varphi_0, \psi_0)\eta(0) + \int_0^T E_{\mathrm{tot}}(\mathbf{v}(t), \varphi(t), \psi(t))\eta(t)\mathrm{d}t \geqq \int_0^T \mathcal{D}(t)\eta(t)\mathrm{d}t$$

for all $\eta \in W^{1,1}(0, T)$ with $\eta \geqq 0$ and $\eta(T) = 0$. In view of Lemma B.6 we then arrive at the energy inequality (3.11).

The proof of Theorem 3.2 is now complete.

4. Proof of Theorem 2.2

We are now in a position to prove our main result Theorem 2.2 by taking advantage of the existence of a solution to the approximating problem studied in Section 3.

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4.1. An Auxiliary Problem with Singular Bulk Potential

We first consider a regularized version of the original problem (1.1)–(1.5) subject to boundary and initial conditions (1.8)–(1.12), with two-parameter viscous regularizing terms, that is, $\varepsilon, \sigma > 0$.

Step 1 (*Construction of solutions to an approximating problem with a regular potential*). On account of Assumption 1 and following [34], we can construct a smooth monotone sequence $\{f_{0\varepsilon}\} \subset C^2(\mathbb{R})$, approximating the singular part of the potential f_0 on compact subintervals of $(-1, 1)$, satisfying (3.2) as well as $f_{0\varepsilon}(0) = 0$. Moreover,

$$|f_{0\varepsilon}(s)| \leqq |f_0(s)|, \quad |F_{0\varepsilon}(s)| \leqq |F_0(s)|, \quad \forall s \in (-1, 1), \tag{4.1}$$

and

$$\lim_{\varepsilon \to 0^+} f_{0\varepsilon}(s) = f_0(s), \quad \lim_{\varepsilon \to 0^+} F_{0\varepsilon}(s) = F_0(s), \quad \forall s \in (-1, 1). \tag{4.2}$$

On the other hand, we replace the linear density function ρ (see Assumption 1) by a smooth nonlinear extension $\widetilde{\rho} : \mathbb{R} \to \mathbb{R}^+$, satisfying

$$\widetilde{\rho}(s) = \rho(s), \quad \forall s \in [-1, 1], \tag{4.3}$$

$$0 < m_* \leqq \widetilde{\rho}(r) \leqq M_*, \quad \left|\widetilde{\rho}^{(j)}(r)\right| \leqq C_j, \quad j = 1, 2 \tag{4.4}$$

for some $C_1, C_2, m_*, M_* > 0$. It is easy to verify that the approximations $f_{0\varepsilon} - c_F r$ and $\widetilde{\rho}$ satisfy the conditions of Theorem 3.2 (cf. Assumption 2).

After the above preparations, in the previous auxiliary system (3.4)–(3.9), we now replace the potential $f(r)$ therein by $f_{0\varepsilon}(r) - c_F r$ and replace the density function ρ by $\widetilde{\rho}$ constructed above (then dropping the tilde from $\widetilde{\rho}$ for the simplicity of notation). For the sake of simplicity, below we set the regularizing parameters

$$\varepsilon = \sigma > 0.$$

Under above choices for the regularized system with a regular potential, for any initial data $\mathbf{v}_0 \in \mathbb{H}$, $(\varphi_0, \psi_0) \in V^1$ such that $F_0(\varphi_0) \in L^1(\Omega)$, $F_0(\psi_0) \in L^1(\Gamma)$, it follows from Theorem 3.2 that there exists a global weak solution $\big(\mathbf{v}_{\sigma,\varepsilon}, \mu_{\sigma,\varepsilon}, \varphi_{\sigma,\varepsilon}, \psi_{\sigma,\varepsilon}\big)$ to the corresponding approximating problem (3.4)–(3.9) in the sense of Definition 3.1, which also satisfies the energy inequality (3.11).

Step 2 (*Passage to the limit as $\varepsilon \to 0^+$, the case of singular potential*). Our next aim is to pass to the limit with respect to $\varepsilon \to 0^+$ (that is, the approximating parameter for the singular potential f_0) with fixed regularizing parameters $\varepsilon = \sigma > 0$.

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The energy inequality (3.11) implies the following uniform (in ε) bounds (cf. (3.57)):

$$\begin{cases} \mathbf{v}_{\sigma,\varepsilon} & \text{is bounded in } L^2(0,T;\mathbb{H}^1) \text{ and in } L^\infty(0,T;\mathbb{H}), \\ \nabla\mu_{\sigma,\varepsilon} & \text{is bounded in } L^2(0,T;\mathbb{L}^2(\Omega)), \\ \mathcal{L}\left(\psi_{\sigma,\varepsilon}\right) & \text{is bounded in } L^2(0,T;L^2(\Gamma)), \\ \left(\varphi_{\sigma,\varepsilon},\psi_{\sigma,\varepsilon}\right) & \text{is bounded in } L^\infty(0,T;V^1), \\ F_{0\varepsilon}\left(\varphi_{\sigma,\varepsilon}\right) & \text{is bounded in } L^\infty(0,T;L^1(\Omega)), \\ G\left(\psi_{\sigma,\varepsilon}\right) & \text{is bounded in } L^\infty(0,T;L^1(\Gamma)), \\ \int_0^T \left|\int_\Omega \mu_{\sigma,\varepsilon}\mathrm{d}x\right| \mathrm{d}t \leqq Q(T), \end{cases} \tag{4.5}$$

for certain monotone function $Q:\mathbb{R}^+\to\mathbb{R}^+$ independent of σ,ε. Indeed, choosing the test function $\xi=1$ in (3.5), we obtain that

$$\int_\Omega \varphi_{\sigma,\varepsilon}(t)\,\mathrm{d}x = \int_\Omega \varphi_0 \mathrm{d}x,$$

and then the last estimate in (4.5) follows by a similar argument, as exploited in (3.44). Then following the same argument as in the proof of Step 1 of [34, Section 7, Theorem 3.5], we obtain that

$$f_{0\varepsilon}\left(\varphi_{\sigma,\varepsilon}\right) \quad \text{is bounded in } L^2(0,T;L^1(\Omega)), \tag{4.6}$$

$$\partial_t\varphi_{\sigma,\varepsilon} \quad \text{is bounded in } L^2(0,T;(H^1(\Omega))^*), \tag{4.7}$$

$$\mu_{\sigma,\varepsilon} \quad \text{is bounded in } L^2(0,T;H^1(\Omega)). \tag{4.8}$$

According to the assumptions (2.4)–(2.5), it is easy to verify that

$$f_{0\varepsilon}'(s)-\delta(f_{0\varepsilon}(s))^2 \geqq -C_{\delta,M}, \qquad \forall\, s\in\mathbb{R}\backslash[-M,M],$$

$$f_{0\varepsilon}(s)(g(s)+\zeta s) \geqq -C_M, \qquad \forall\, s\in\mathbb{R}\backslash[-M,M],$$

with constants $C_{\delta,M}, C_M>0$ independent of $\varepsilon\in(0,\varepsilon_0]$ for some $\varepsilon_0>0$. Then an argument similar to Step 2 of [34, Section 7, Theorem 3.5] yields

$$f_{0\varepsilon}\left(\varphi_{\sigma,\varepsilon}\right) \quad \text{is bounded in } L^2(0,T;L^2(\Omega)), \tag{4.9}$$

$$F_{0\varepsilon}\left(\psi_{\sigma,\varepsilon}\right) \quad \text{is bounded in } L^\infty(0,T;L^1(\Gamma)), \tag{4.10}$$

provided that the additional assumption $F_0(\psi_0)\in L^1(\Gamma)$ holds.

Using these bounds, we can pass to the limit up to a subsequence, as $\varepsilon\to 0^+$, to get

$$\mathbf{v}_{\sigma,\varepsilon} \rightharpoonup \mathbf{v}_\sigma \quad \text{in } L^2(0,T;\mathbb{H}^1), \tag{4.11}$$

$$\mathbf{v}_{\sigma,\varepsilon} \rightharpoonup^* \mathbf{v}_\sigma \quad \text{in } L^\infty(0,T;\mathbb{H}) \cong \left(L^1(0,T;\mathbb{H})\right)^*, \tag{4.12}$$

$$\left(\varphi_{\sigma,\varepsilon},\psi_{\sigma,\varepsilon}\right) \rightharpoonup^* (\varphi_\sigma,\psi_\sigma) \quad \text{in } L^\infty(0,T;V^1) \cong \left(L^1(0,T;(V^1)^*)\right)^*, \tag{4.13}$$

$$\mu_{\sigma,\varepsilon} \rightharpoonup \mu_\sigma \quad \text{in } L^2(0,T;H^1(\Omega)), \tag{4.14}$$

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$$\nabla \mu_{\sigma,\varepsilon} \rightharpoonup \nabla \mu_\sigma \ \text{ in } \ L^2(0,T;\mathbb{L}^2(\Omega)), \tag{4.15}$$

$$\mathcal{L}\left(\psi_{\sigma,\varepsilon}\right) \rightharpoonup \mathcal{L}\left(\psi_\sigma\right) \ \text{ in } \ L^2(0,T;L^2(\Gamma)). \tag{4.16}$$

By the growth assumption on g, we have

$$g\left(\psi_{\sigma,\varepsilon}\right) \ \text{is bounded in } L^2\left(0,T;L^2(\Gamma)\right). \tag{4.17}$$

This together with (4.9) and $\sigma\partial_t\varphi_{\sigma,\varepsilon} \in L^2(0,T;L^2(\Omega))$ allows us to conclude the following estimate:

$$\left(\varphi_{\sigma,\varepsilon},\psi_{\sigma,\varepsilon}\right) \ \text{is bounded } \ \text{in } \ L^2(0,T;V^2), \tag{4.18}$$

by the same argument as for (3.59) with the aid of Lemma B.4. Due to (4.5)–(4.8), we also have $\partial_t\psi_{\sigma,\varepsilon}$ is bounded (uniformly in ε) in $L^2\left(0,T;L^2(\Gamma)\right)$, since

$$\mathbf{v}_{\sigma,\varepsilon} \text{ is bounded in } L^q\left(0,T;\mathbb{W}^{1,q}(\Omega)\right), \quad \text{for some } q > 2d, \tag{4.19}$$

uniformly with respect to $\varepsilon > 0$. Hence, Lemma B.1 yields that

$$\left(\varphi_{\sigma,\varepsilon},\psi_{\sigma,\varepsilon}\right) \longrightarrow \left(\varphi_\sigma,\psi_\sigma\right) \ \text{in } \ L^2(0,T;V^{2-s}), \quad \text{for any } s \in (0,1/2), \tag{4.20}$$

which also implies, due to (4.13) and (4.18), the improved strong convergence

$$\left(\varphi_{\sigma,\varepsilon},\psi_{\sigma,\varepsilon}\right) \longrightarrow \left(\varphi_\sigma,\psi_\sigma\right) \ \text{in } \ L^r(0,T;H^1(\Omega)\times H^1(\Gamma)), \quad \forall r \in [2,\infty) \tag{4.21}$$

and

$$\left(\varphi_{\sigma,\varepsilon},\psi_{\sigma,\varepsilon}\right) \longrightarrow \left(\varphi_\sigma,\psi_\sigma\right) \ \text{in } L^2\left(0,T;L^\infty(\Omega)\times L^\infty(\Gamma)\right). \tag{4.22}$$

In fact, by interpolation in (4.20) together with (4.13) we can get even stronger convergence results, namely,

$$\nabla\varphi_{\sigma,\varepsilon} \to \nabla\varphi_\sigma \quad \text{in } L^4(0,T;\mathbb{L}^{\frac{6}{2+s}}(\Omega)) \cap L^{4(1-s)}(0,T;\mathbb{L}^3(\Omega)), \tag{4.23}$$

$$\nabla\varphi_{\sigma,\varepsilon} \to \nabla\varphi_\sigma \quad \text{in } L^p(0,T;\mathbb{L}^p(\Omega)), \quad \text{with } p := (10-4s)/3, \tag{4.24}$$

$$\nabla_{\boldsymbol{\tau}}\psi_{\sigma,\varepsilon} \to \nabla_{\boldsymbol{\tau}}\psi_\sigma \quad \text{in } L^4(0,T;\mathbb{L}^{\frac{4}{1+s}}(\Gamma)) \cap L^{4(1-s)}(0,T;\mathbb{L}^4(\Gamma)), \tag{4.25}$$

for any $s \in (0,1/2)$. Owing to (4.9), the pointwise convergence of $\varphi_{\sigma,\varepsilon}$ due to (4.20) and the assumptions on f_0 (see Assumption 1), we can conclude that (cf. [53, Section 3])

$$|\varphi_\sigma| < 1 \quad \text{almost everywhere in } Q_T.$$

Then by (4.10) and (4.20) we also have

$$|\psi_\sigma| \leqq 1 \quad \text{almost everywhere on } \Sigma_T.$$

From the above facts, (4.9), (4.10) and the convergence of $\varphi_{\sigma,\varepsilon}$ and $\psi_{\sigma,\varepsilon}$ almost everywhere in Q_T and on Σ_T, respectively, we also deduce that

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$$f_{0\varepsilon}\left(\varphi_{\sigma,\varepsilon}\right) \rightharpoonup f_0\left(\varphi_\sigma\right) \quad \text{in } L^2\left(0,T;L^2\left(\Omega\right)\right), \tag{4.26}$$

$$g\left(\psi_{\sigma,\varepsilon}\right) \rightharpoonup g\left(\psi_\sigma\right) \quad \text{in } L^2(0,T;L^2\left(\Gamma\right)), \tag{4.27}$$

$$F_{0\varepsilon}\left(\psi_{\sigma,\varepsilon}\right) \rightharpoonup^* F_0\left(\psi_\sigma\right) \quad \text{in } L^\infty(0,T;L^1\left(\Gamma\right)), \tag{4.28}$$

since $F_{0\varepsilon}$ and F_0 are (strictly) convex functions, obeying (4.1)–(4.2).

In view of the convergence relations in (4.11)–(4.16) and (4.20)–(4.27), we may pass to the limit in a straightforward manner as in [34, Section 5, pp. 29–31], to deduce that the limit function $(\mathbf{v}_\sigma, \mu_\sigma, \varphi_\sigma, \psi_\sigma)$, obtained from the limit procedure in $\varepsilon \to 0^+$, satisfies equations (3.5)–(3.7).

The final step consists in showing that the limit function $\mathbf{v}_\sigma$ also satisfies a suitable equation for the fluid velocity. This is the most crucial point. As in the proof of Theorem 3.2 (now with $\sigma = \varepsilon > 0$), we require to show that, along a suitable subsequence, it holds that $\mathbf{v}_{\sigma,\varepsilon} \to \mathbf{v}_\sigma$ in $L^2(0,T;\mathbb{L}^2(\Omega))$ at least. To this end, it suffices to show exactly, as in the foregoing proof (now with $\sigma = \varepsilon > 0$), that

$$\partial_t(\mathbb{P}(\rho\left(\varphi_{\sigma,\varepsilon}\right)\mathbf{v}_{\sigma,\varepsilon})) \text{ is bounded in } L^1(0,T;\mathbb{H}^{-3/2-\delta}) \oplus L^{\frac{q}{q-1}}\left(0,T;\left(\mathbb{W}^{1,q}(\Omega)\right)^*\right) \tag{4.29}$$

for any $\delta \geqq 1/4$, $q > 2d$. However this bound requires once again some uniform bounds of the nonlinear terms that occur in the equation for $\mathbf{v}_{\sigma,\varepsilon}$. Due to the previous bounds in (4.5)–(4.18), we have, exactly[3] as in (3.79)–(3.80), that

$$\begin{cases} \rho\left(\varphi_{\sigma,\varepsilon}\right)\mathbf{v}_{\sigma,\varepsilon}\otimes\mathbf{v}_{\sigma,\varepsilon} & \text{is bounded in } \; L^2(0,T;L^{3/2}(\Omega)^{d\times d}), \\ \mathbf{v}_{\sigma,\varepsilon}\otimes\nabla\mu_{\sigma,\varepsilon} & \text{is bounded in } \; L^{8/7}(0,T;L^{4/3}(\Omega)^{d\times d}), \\ \mu_{\sigma,\varepsilon}\nabla\varphi_{\sigma,\varepsilon} & \text{is bounded in } \; L^2(0,T;\mathbb{L}^{3/2}(\Omega)), \\ \mathcal{L}\left(\psi_{\sigma,\varepsilon}\right)\nabla_{\boldsymbol{\tau}}\psi_{\sigma,\varepsilon} & \text{is bounded in } \; L^{8/7}(0,T;\mathbb{L}^{8/7}(\Gamma)). \end{cases} \tag{4.30}$$

Thus, it remains to bound the following term uniformly in ε:

$$\left\langle R_\sigma \mathbf{v}_{\sigma,\varepsilon}, \mathbf{w}\right\rangle = -\int_{Q_T} m\left(\varphi_{\sigma,\varepsilon}\right)\left(\nabla\rho'\left(\varphi_{\sigma,\varepsilon}\right)\cdot\nabla\mu_{\sigma,\varepsilon}\right)\mathbf{v}_{\sigma,\varepsilon}\cdot\mathbf{w}\,\mathrm{d}x\,\mathrm{d}t, \tag{4.31}$$

for all $\mathbf{w} \in C_0^\infty(0,T;\mathbb{H}^{3/2+\delta}\cap\mathbb{W}^{1,q}(\Omega))$. Since $\rho'' \in L^\infty((0,T)\times\Omega)$ and

$$\nabla\varphi_{\sigma,\varepsilon} \in L^4\left(0,T;\mathbb{L}^3\left(\Omega\right)\right), \; \nabla\mu_{\sigma,\varepsilon} \in L^2\left(0,T;\mathbb{L}^2\left(\Omega\right)\right)$$

are bounded as $\varepsilon \to 0^+$, it also follows that $R_\sigma\mathbf{v}_{\sigma,\varepsilon} \in L^1(0,T;\mathbb{H}^{-3/2-\delta})$ is uniformly bounded with respect to $\varepsilon > 0$ because of (4.19). Hence, we can conclude the estimate (4.29) on time derivative. As a consequence, owing to (4.29) with the help of Lemma B.1, we deduce once again as in (3.84)–(3.90) that

$$\mathbf{v}_{\sigma,\varepsilon} \to \mathbf{v}_\sigma \text{ in } L^2(0,T;\mathbb{W}^{1,4}\left(\Omega\right)) \hookrightarrow L^2(0,T;\mathbb{L}^\infty\left(\Omega\right)). \tag{4.32}$$

[3] Note that the bounds in (3.79)–(3.81) are already uniform in $\sigma = \varepsilon > 0$, $\varepsilon \in [0, 1]$.

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This strong convergence together with (4.19) yields yet by interpolation that

$$\mathbf{v}_{\sigma,\varepsilon} \to \mathbf{v}_\sigma \text{ in } L^{5+\delta}(0,T;\mathbb{L}^{5+\delta}(\Omega)), \tag{4.33}$$

for some sufficiently small $\delta = \delta(q) > 0$ for $q > 2d$ sufficiently large. Then the passage to the limit as $\varepsilon \to 0^+$ in all nonlinear terms that occur in the equation for $\mathbf{v}_{\sigma,\varepsilon}$, with the exception of the one involving the source term $R_\sigma \mathbf{v}_{\sigma,\varepsilon}$, is easy on account of the same arguments used in (3.88)–(3.89). On the other hand, since we have shown that $|\varphi_\sigma| < 1$ almost everywhere in Q_T, then the nonlinear extended density function $\rho(r)$ constructed in Step 1 is indeed linear for $r \in [-1,1]$. As a consequence, it now follows from (4.24), (4.33) and the weak convergence (4.15) that

$$\left\langle R_\sigma \mathbf{v}_{\sigma,\varepsilon}, \mathbf{w}\right\rangle \longrightarrow 0 \quad \text{for all } \mathbf{w} \in C_0^\infty\left(0,T;\mathbb{C}_{\text{div}}^\infty\left(\overline{\Omega}\right)\right), \tag{4.34}$$

as long as we fix a sufficiently small $s \in (0,1/2)$ from (4.24) satisfying

$$\frac{3}{10-4s} + \frac{1}{5+\delta} \leqq \frac{1}{2}. \tag{4.35}$$

Since (4.33) holds for some fixed $\delta > 0$, we infer from (4.34) that $(\mathbf{v}_\sigma, \mu_\sigma, \varphi_\sigma, \psi_\sigma)$ is indeed a weak solution in the sense of Definition 3.1 with now a trivial external source

$$R_\sigma = 0.$$

The energy inequality (3.11) associated with $(\mathbf{v}_\sigma, \mu_\sigma, \varphi_\sigma, \psi_\sigma)$ can be proven exactly as before, taking advantage of the convexity properties of F_0, $F_{0\varepsilon}$, (4.1)–(4.2) and the strong convergence results (4.20)–(4.22). Besides, the initial conditions $\mathbf{v}_\sigma(0) = \mathbf{v}_0$, $\varphi_\sigma(0) = \varphi_0$ and $\psi_\sigma(0) = \psi_0$, can be verified in a similar fashion as in the proof of Theorem 3.2.

4.2. Passage to the Limit as $\varepsilon = \sigma \to 0^+$

To complete the proof of Theorem 2.2, it remains to pass to the limit as $\varepsilon = \sigma \to 0^+$ in the above approximating problem.

As a consequence of the energy inequality for $(\mathbf{v}_\sigma, \mu_\sigma, \varphi_\sigma, \psi_\sigma)$ (cf. (3.11)), we again have the uniform (in $\sigma = \varepsilon$) bounds (4.5)–(4.10) for $(\mathbf{v}_\sigma, \mu_\sigma, \varphi_\sigma, \psi_\sigma)$. The passage to the limit as $\varepsilon = \sigma \to 0^+$ is simply based on these estimates and we only briefly mention some details at the expense of repeating several earlier arguments.

To this end, for a proper subsequence, we have, once again,

$$\mathbf{v}_\sigma \rightharpoonup \mathbf{v} \quad \text{in } L^2(0,T;\mathbb{H}^1), \tag{4.36}$$

$$\mathbf{v}_\sigma \rightharpoonup^* \mathbf{v} \quad \text{in } L^\infty(0,T;\mathbb{H}) \cong \left(L^1(0,T;\mathbb{H})\right)^*, \tag{4.37}$$

$$(\varphi_\sigma, \psi_\sigma) \rightharpoonup^* (\varphi, \psi) \quad \text{in } L^\infty(0,T;V^1) \cong \left(L^1(0,T;(V^1)^*)\right)^*, \tag{4.38}$$

$$\mu_\sigma \rightharpoonup \mu \quad \text{in } L^2(0,T;H^1(\Omega)), \tag{4.39}$$

$$\nabla\mu_\sigma \rightharpoonup \nabla\mu \quad \text{in } L^2(0,T;\mathbb{L}^2(\Omega)), \tag{4.40}$$

$$\mathcal{L}(\psi_\sigma) \rightharpoonup \mathcal{L}(\psi) \quad \text{in } L^2(0,T;L^2(\Gamma)). \tag{4.41}$$

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Employing the same arguments from [34, Section 7, Theorem 3.5], we obtain

$$f_0(\varphi_\sigma) \quad \text{is bounded in } L^2(0,T;L^1(\Omega)) \tag{4.42}$$

as well as

$$\partial_t \varphi_\sigma \text{ is bounded in } L^2(0,T;(H^1(\Omega))^*) \tag{4.43}$$

and

$$\partial_t \psi_\sigma \text{ is bounded in } \begin{cases} L^{4/3}\left(0,T;L^2(\Gamma)\right), & \text{if } d=3, \\ L^{\frac{4s}{3s-2}}\left(0,T;L^2(\Gamma)\right), & \text{if } d=2,\ s>2. \end{cases} \tag{4.44}$$

The bound (4.44) is weaker than the one we used in Section 4.1, since we can no longer rely on (4.19). Furthermore, we see from [34, Section 7, Theorem 3.5] that

$$f_0(\varphi_\sigma) \quad \text{is bounded in } L^2(0,T;L^2(\Omega)), \tag{4.45}$$

$$F_0(\psi_\sigma) \quad \text{is bounded in } L^\infty(0,T;L^1(\Gamma)). \tag{4.46}$$

Then we recover once again, as for (4.20), a strong convergence on $(\varphi_\sigma, \psi_\sigma)$:

$$(\varphi_\sigma, \psi_\sigma) \longrightarrow (\varphi, \psi) \text{ in } L^2(0,T;V^{2-s}), \quad \text{for any } s \in (0,1/2). \tag{4.47}$$

Due to the pointwise convergence of $\varphi_\sigma \to \varphi$ in Q_T, the continuity of $f_0 \in C(-1,1)$ and the fact $|\varphi_\sigma| < 1$ almost everywhere in Q_T, it holds that

$$f_0(\varphi_\sigma) \to f_0(\varphi) \quad \text{almost everywhere in } Q_T.$$

Then the pointwise convergence of $f_0(\varphi_\sigma)$, together with the bound (4.45), yields, up to a subsequence that

$$f_0(\varphi_\sigma) \rightharpoonup f_0(\varphi) \quad \text{in } L^2\left(0,T;L^2(\Omega)\right). \tag{4.48}$$

Also, the weak convergence for the nonlinear boundary term

$$g(\psi_\sigma) \rightharpoonup g(\psi) \quad \text{in } L^2\left(0,T;L^2(\Gamma)\right)$$

follows from a similar argument as to that for (3.75).

The strong convergence

$$\mathbf{v}_\sigma \to \mathbf{v} \quad \text{in } L^2(0,T;\mathbb{L}^2(\Omega))$$

in fact requires no changes to the bounds in (4.30), since these were already uniform in σ, $\varepsilon > 0$ and merely a consequence of (4.36)–(4.41). Indeed, since the additional (highly nonlinear) source R_σ is no longer present on the right-hand side for the equation of $\mathbf{v}_\sigma$, the uniform bound in (4.29) is readily available as

$$\partial_t(\mathbb{P}(\rho(\varphi_\sigma)\mathbf{v}_\sigma)) \text{ is bounded in } L^1(0,T;\mathbb{H}^{-3/2-\delta}) \oplus L^{\frac{q}{q-1}}\left(0,T;\left(\mathbb{W}^{1,q}(\Omega)\right)^*\right) \tag{4.49}$$

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for some $q > 2d$. Hence, once again we can reach the necessary strong convergence $\mathbf{v}_\sigma \to \mathbf{v}$ by virtue of (3.84)–(3.87). Next, because, as $\sigma = \varepsilon \to 0^+$, it holds that

$$\sigma \partial_t \varphi_\sigma \to 0 \qquad \text{in } L^2\left(0, T; L^2(\Omega)\right),$$

$$\varepsilon\left(|D\mathbf{v}|^{q-2} D\mathbf{v} + |\mathbf{v}|^{q-2}\mathbf{v}\right) \to 0 \quad \text{in } L^{\frac{q}{q-1}}\left(0, T; \left(\mathbb{W}^{1,q}(\Omega)\right)^*\right),$$

one can easily show that $(\mathbf{v}, \mu, \varphi, \psi)$ is a weak solution in the sense of Definition 2.1 with now a zero source term $R = 0$.

Finally, the proof of the energy inequality (2.22) and the equalities on initial data

$$\mathbf{v}(0) = \mathbf{v}_0, \quad \varphi(0) = \varphi_0, \quad \psi(0) = \psi_0$$

follow verbatim from the proof of Theorem 3.2, only with some minor inessential modifications and arguments. We skip these obvious details.

The proof of Theorem 2.2 is complete.

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Conflict of interest The authors declare that they have no conflict of interest.

Appendix A. Derivation of the Model via Variational Principles

In this section, we derive the diffuse interface model (1.1)–(1.5) subject to (1.8)–(1.12) by employing fundamental postulations of thermodynamics, in particular, the Onsager's variational principle (see [55,56,59]).

Following the argument in [7], we adopt an order parameter $\varphi\ (= u_2 - u_1)$ as the difference of the volume fractions $u_j\ (j = 1, 2)$ of the two liquids involved. We assume $u_1 + u_2 = 1$ and the averaged density of the mixture can be expressed as an affine function in terms of φ such that

$$\rho(\varphi) = \frac{\rho_2 - \rho_1}{2}\varphi + \frac{\rho_1 + \rho_2}{2}, \tag{A.1}$$

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where ρ_1 and ρ_2 are the specific densities of liquid 1 and 2, respectively. In addition, we choose the volume averaged velocity

$$\mathbf{v} := u_1\mathbf{v}_1 + u_2\mathbf{v}_2 = \frac{1-\varphi}{2}\mathbf{v}_1 + \frac{1+\varphi}{2}\mathbf{v}_2, \tag{A.2}$$

where $\mathbf{v}_j$ $(j = 1, 2)$ is the individual velocity for component j. A direct calculation implies that

$$\operatorname{div} \mathbf{v} = 0. \tag{A.3}$$

Then the balance laws for mass and linear momentum can be given as the following set of partial differential equations in terms of φ and $\mathbf{v}$ (see [7, Section 2]):

$$\rho\partial_t \mathbf{v} + \left(\left(\rho\mathbf{v} + \frac{\partial\rho}{\partial\varphi}\mathbf{J}_\varphi\right)\cdot\nabla\right)\mathbf{v} - \operatorname{div}\mathbf{S} + \nabla p = \mathbf{K}, \tag{A.4}$$

$$\partial_t\varphi + \mathbf{v}\cdot\nabla\varphi + \operatorname{div}\mathbf{J}_\varphi = 0, \tag{A.5}$$

with $\rho(\cdot)$ being exactly as in (A.1) and

$$\mathbf{J}_\varphi = \left(\frac{\rho_1+\rho_2}{2}\right)^{-1}\mathbf{J}$$

being a rescaled mass flux. Here, $\mathbf{S}$ denotes the symmetric stress tensor and $\mathbf{K}$ stands for the force density. These equations hold in a space-time cylinder Q_T with $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$ being the domain where this process takes place *in the absence of any dynamical effects at the solid boundary* $\Gamma = \partial\Omega$. Conservation of mass requires that the normal component of $\mathbf{J}_\varphi$ is zero, while an impenetrable boundary Γ requires that the normal component of the velocity $\mathbf{v}$ is also zero, namely,

$$\mathbf{J}_\varphi\cdot\mathbf{n} = 0, \quad \mathbf{v}\cdot\mathbf{n} = 0, \quad \text{on } \Gamma.$$

Next, concerning the free energy of the system, we choose

$$E_{\text{free}} := \int_\Omega \Phi_b(\varphi, \nabla\varphi)\mathrm{d}x + \int_\Gamma \Phi_s(\varphi, \nabla_{\boldsymbol{\tau}}\varphi)\mathrm{d}S$$

with $\Phi_b(z, p) = \Phi_b^1(z) + \Phi_b^2(p)$, and $\Phi_s(z, p) = \Phi_s^1(z) + \Phi_s^2(p)$. Here, the second term represents an interfacial free energy per unit surface area at the fluid-solid interface, which is a function of the local composition. Then the total energy is given by the sum of kinetic and free energies such that

$$\mathcal{F} := \int_\Omega \frac{1}{2}\rho(\varphi)|\mathbf{v}|^2\mathrm{d}x + \int_\Omega \Phi_b(\varphi, \nabla\varphi)\mathrm{d}x + \int_\Gamma \Phi_s(\varphi, \nabla_{\boldsymbol{\tau}}\varphi)\mathrm{d}S.$$

The time derivative of the free energy is given by

$$\begin{aligned}\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t} &= \frac{1}{2}\int_\Omega \frac{\partial\rho}{\partial\varphi}|\mathbf{v}|^2\partial_t\varphi\mathrm{d}x + \int_\Omega \frac{\partial\Phi_b}{\partial\varphi}\partial_t\varphi\mathrm{d}x \\ &\quad - \int_\Omega \operatorname{div}\left(\frac{\partial\Phi_b}{\partial\nabla\varphi}\right)\partial_t\varphi\mathrm{d}x + \int_\Omega \rho(\varphi)\mathbf{v}\cdot\partial_t\mathbf{v}\mathrm{d}x\end{aligned}$$

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$$+\int_\Gamma \left(\frac{\partial \Phi_s}{\partial \varphi} + \frac{\partial \Phi_b}{\partial \nabla\varphi}\cdot \mathbf{n}\right)\partial_t\varphi \mathrm{d}S$$
$$-\int_\Gamma \mathrm{div}_{\boldsymbol{\tau}}\left(\frac{\partial \Phi_s}{\partial \nabla_{\boldsymbol{\tau}}\varphi}\right)\partial_t\varphi \mathrm{d}S, \tag{A.6}$$

which follows by integration by parts (using the divergence theorems in Ω and on Γ, respectively) in the third and last summands of $\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t}$. Here $\mathrm{div}_{\boldsymbol{\tau}}$ denotes tangential divergence on Γ. We observe from (A.4) that

$$\partial_t \mathbf{v} = \frac{1}{\rho}\left\{\mathbf{K} + \mathrm{div}\,\mathbf{S} - \left(\left(\rho\mathbf{v} + \frac{\partial\rho}{\partial\varphi}\mathbf{J}_\varphi\right)\cdot\nabla\right)\mathbf{v} - \nabla p\right\}.$$

Inserting this equation and (A.5) into the right-hand side of (A.6), then using integration by parts and $\mathbf{v}\cdot\mathbf{n} = 0$ on Γ, we obtain

$$\begin{aligned}
\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t} &= -\frac{1}{2}\int_\Omega \frac{\partial\rho}{\partial\varphi}|\mathbf{v}|^2(\mathbf{v}\cdot\nabla\varphi + \mathrm{div}\,\mathbf{J}_\varphi)\mathrm{d}x \\
&\quad - \int_\Omega \frac{\partial\Phi_b}{\partial\varphi}(\mathbf{v}\cdot\nabla\varphi + \mathrm{div}\,\mathbf{J}_\varphi)\mathrm{d}x \\
&\quad + \int_\Omega \mathrm{div}\left(\frac{\partial\Phi_b}{\partial\nabla\varphi}\right)(\mathbf{v}\cdot\nabla\varphi + \mathrm{div}\,\mathbf{J}_\varphi)\mathrm{d}x \\
&\quad + \int_\Gamma\left(\frac{\partial\Phi_s}{\partial\varphi} + \frac{\partial\Phi_b}{\partial\nabla\varphi}\cdot\mathbf{n} - \mathrm{div}_{\boldsymbol{\tau}}\left(\frac{\partial\Phi_s}{\partial\nabla_{\boldsymbol{\tau}}\varphi}\right)\right)\partial_t\varphi\mathrm{d}S \\
&\quad + \int_\Omega \mathbf{v}\cdot\left\{\mathbf{K} + \mathrm{div}\,\mathbf{S} - \left(\left(\rho\mathbf{v} + \frac{\partial\rho}{\partial\varphi}\mathbf{J}_\varphi\right)\cdot\nabla\right)\mathbf{v} - \nabla p\right\}\mathrm{d}x \\
&= -\int_\Omega \mathbf{v}\cdot\nabla\varphi\mu_\varphi\mathrm{d}x + \int_\Omega \mathbf{J}_\varphi\cdot\nabla\mu_\varphi\mathrm{d}x - \int_\Omega D\mathbf{v} : \mathbf{S}\mathrm{d}x \\
&\quad + \int_\Gamma \mathcal{L}_\varphi\partial_t\varphi\mathrm{d}S + \int_\Omega \mathbf{v}\cdot\mathbf{K}\mathrm{d}x + \int_\Gamma (\mathbf{S}\cdot\mathbf{n})_{\boldsymbol{\tau}}\cdot\mathbf{v}_{\boldsymbol{\tau}}\mathrm{d}S.
\end{aligned} \tag{A.7}$$

Here we have used the following fact:

$$\int_\Omega \mathbf{v}\cdot\left(\left(\rho\mathbf{v} + \frac{\partial\rho}{\partial\varphi}\mathbf{J}_\varphi\right)\cdot\nabla\right)\mathbf{v}\mathrm{d}x = -\frac{1}{2}\int_\Omega \frac{\partial\rho}{\partial\varphi}|\mathbf{v}|^2\left(\mathbf{v}\cdot\nabla\varphi + \mathrm{div}\mathbf{J}_\varphi\right)\mathrm{d}x,$$

which, as a consequence of the no-flux boundary conditions $\mathbf{J}_\varphi\cdot\mathbf{n} = \mathbf{v}\cdot\mathbf{n} = 0$ on Γ, follows easily from integration by parts. Moreover, we have set

$$\mu_\varphi := -\mathrm{div}\left(\frac{\partial\Phi_b}{\partial\nabla\varphi}\right) + \frac{\partial\Phi_b}{\partial\varphi},$$
$$\mathcal{L}_\varphi := \frac{\partial\Phi_s}{\partial\varphi} + \frac{\partial\Phi_b}{\partial\nabla\varphi}\cdot\mathbf{n} - \mathrm{div}_{\boldsymbol{\tau}}\left(\frac{\partial\Phi_s}{\partial\nabla_{\boldsymbol{\tau}}\varphi}\right)$$

in order to denote the chemical potentials corresponding to φ in the bulk Ω and on the solid boundary Γ, respectively. On the other hand, the work rate $\frac{\mathrm{d}\mathcal{W}}{\mathrm{d}t}$ is due to the work done by the flow to the fluid–fluid interface and is defined by

$$\frac{\mathrm{d}\mathcal{W}}{\mathrm{d}t} = -\int_\Omega(\mathbf{v}\cdot\nabla\varphi)\mu_\varphi\mathrm{d}x + \int_\Omega \mathbf{v}\cdot\mathbf{K}\mathrm{d}x - \int_\Gamma(\mathbf{v}_{\boldsymbol{\tau}}\cdot\nabla_{\boldsymbol{\tau}}\varphi)\mathcal{L}_\varphi\mathrm{d}S, \tag{A.8}$$

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where $\mu_\varphi \nabla\varphi$ is the capillary force density and $\mathcal{L}_\varphi \nabla_{\boldsymbol{\tau}}\varphi$ is the uncompensated Young stress (see [58,59]), both being the “elastic" interfacial forces. We recall that $\mathbf{v}_{\boldsymbol{\tau}} = \mathbf{v} - (\mathbf{v}\cdot\mathbf{n})\,\mathbf{n}$ is defined as the tangential fluid velocity at the solid boundary Γ measured relative to the wall. Then the rate of change of the mechanical work becomes

$$\frac{\mathrm{d}\mathcal{W}}{\mathrm{d}t} = \int_\Omega \mathbf{v}\cdot\mathbf{K}_{\mathrm{grav}}\mathrm{d}x - \int_\Gamma (\mathbf{v}_{\boldsymbol{\tau}}\cdot\nabla_{\boldsymbol{\tau}}\varphi)\mathcal{L}_\varphi \mathrm{d}S$$

if $\mathbf{K} = \mu_\varphi\nabla\varphi + \mathbf{K}_{\mathrm{grav}}$, where $\mathbf{K}_{\mathrm{grav}}$ denotes the gravitational force.

To derive a closed system for (A.4)–(A.5), it remains to determine the flux $\mathbf{J}_\varphi$ and the stress tensor $\mathbf{S}$. For this purpose, we introduce the dissipation functional (see [59])

$$\Psi(\mathbf{J}_\varphi, \mathbf{S}, \partial_t^{\boldsymbol{\tau}}\varphi, \mathbf{v}) := \int_\Omega \left\{ \frac{|\mathbf{J}_\varphi|^2}{2m(\varphi)} + \frac{|\mathbf{S}|^2}{4\nu(\varphi)} \right\} \mathrm{d}x + \int_\Gamma \left\{ \frac{\beta(\varphi)}{2} |\mathbf{v}_{\boldsymbol{\tau}}|^2 + \frac{\left|\partial_t^{\boldsymbol{\tau}}\varphi\right|^2}{2l_0(\varphi)} \right\} \mathrm{d}S. \tag{A.9}$$

Here, m plays the role of mobility, ν is the shear viscosity and β is a slip coefficient relative to the solid boundary Γ, all may depend on the local concentration. There are four physically distinct sources of the dissipation in (A.9), the first and second summands represent the composition diffusion in the bulk and shear viscosity in the bulk, respectively. The third summand arises from the assumption of fluid slipping at the solid surface Γ, while the last summand accounts for the composition relaxation at the solid surface with a relaxation parameter l_0, where $\partial_t^{\boldsymbol{\tau}}\varphi = \partial_t\varphi + \mathbf{v}_{\boldsymbol{\tau}}\cdot\nabla_{\boldsymbol{\tau}}\varphi$. Notice that each term that contributes to Ψ is positive definite and quadratic in a rate that arises from the displacement from the equilibrium. This quadratic dependence follows from the general rule governing entropy production in a thermodynamic process; it directly arises from a linear response to small perturbations away from the equilibrium. Next, we employ Onsager's variational principle (see [55,56]), which postulates that

$$\delta_{(\mathbf{J}_\varphi,\mathbf{S},\mathbf{v},\partial_t^{\boldsymbol{\tau}}\varphi)}\left(\Psi + \frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t}\right) = 0. \tag{A.10}$$

Since Ψ is quadratic in $(\mathbf{J}_\varphi, \mathbf{S}, \mathbf{v}, \partial_t^{\boldsymbol{\tau}}\varphi)$ and $\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t}$ is linear in $(\mathbf{J}_\varphi, \mathbf{S}, \mathbf{v}, \partial_t^{\boldsymbol{\tau}}\varphi)$, using the fact that in (A.7),

$$\int_\Gamma \mathcal{L}_\varphi \partial_t\varphi \mathrm{d}S = \int_\Gamma \mathcal{L}_\varphi \left(\partial_t^{\boldsymbol{\tau}}\varphi - \mathbf{v}_{\boldsymbol{\tau}}\cdot\nabla_{\boldsymbol{\tau}}\varphi\right)\mathrm{d}S,$$

we deduce from (A.7) and (A.9) that the variational principle presented in equation (A.10) gives

$$\mathbf{J}_\varphi = -m(\varphi)\nabla\mu_\varphi \quad \text{and} \quad \mathbf{S} = 2\nu(\varphi)D\mathbf{v},$$

as well as a generalized Navier boundary condition with uncompensated Young stress

$$(\mathbf{S}\cdot\mathbf{n})_{\boldsymbol{\tau}} + \beta(\varphi)\,\mathbf{v}_{\boldsymbol{\tau}} = \mathcal{L}_\varphi\nabla_{\boldsymbol{\tau}}\varphi \quad \text{on } \Gamma.$$

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Similarly, the corresponding Euler–Lagrange equation for minimizing $\Psi + \frac{d\mathcal{F}}{dt}$ with respect to $\partial_t^{\boldsymbol{\tau}}\varphi$ at the solid wall Γ yields the dynamic boundary condition

$$\partial_t^{\boldsymbol{\tau}}\varphi = \partial_t\varphi + \mathbf{v}_{\boldsymbol{\tau}} \cdot \nabla_{\boldsymbol{\tau}}\varphi = -l_0(\varphi)\,\mathcal{L}_\varphi. \tag{A.11}$$

Namely, the relaxation dynamics of the moving contact line at the solid surface is linearly proportional to $\mathcal{L}_\varphi$, which is determined by an advection-reaction equation of Allen–Cahn type.

Remark A.1. In order to simplify the notation, we actually use the same symbol for a function and its trace on the boundary. As it was clarified in [37], we note that the compatibility relation $\partial_t(\mathrm{tr}(\varphi)) = \mathrm{tr}(\partial_t\varphi)$ on Γ, whenever φ is a smooth function, while the right-hand side of such a formula is meaningless in the opposite case. Here in our context, the true meaning of $\partial_t\varphi$ on the boundary should be $\partial_t(\mathrm{tr}(\varphi))$, which is meaningful (at least in a generalized sense) whenever $\varphi \in L^2(0, T; H^1(\Omega))$.

In conclusion, in the absence of any gravitational forces ($\mathbf{K}_{\mathrm{grav}} = 0$), with a density ρ given by (A.1), we end up with the evolution system

$$\begin{cases} \rho\partial_t\mathbf{v} + \left(\left(\rho\mathbf{v} + \dfrac{\partial\rho}{\partial\varphi}\mathbf{J}_\varphi\right)\cdot\nabla\right)\mathbf{v} - \mathrm{div}\,(2\nu(\varphi)\,D\mathbf{v}) + \nabla p = \mu_\varphi\nabla\varphi, & \text{in } Q_T, \\ \mathrm{div}\,\mathbf{v} = 0, & \text{in } Q_T, \\ \partial_t\varphi + \mathbf{v}\cdot\nabla\varphi - \mathrm{div}\left(m(\varphi)\,\nabla\mu_\varphi\right) = 0, & \text{in } Q_T, \\ \mu_\varphi = -\mathrm{div}\left(\dfrac{\partial\Phi_b}{\partial\nabla\varphi}\right) + \dfrac{\partial\Phi_b}{\partial\varphi}, & \text{in } Q_T, \end{cases} \tag{A.12}$$

subject to the boundary conditions

$$\begin{cases} \mathbf{v}\cdot\mathbf{n} = \partial_{\mathbf{n}}\mu_\varphi = 0, & \text{on } \Sigma_T, \\ (2\nu(\varphi)D\mathbf{v}\cdot\mathbf{n})_{\boldsymbol{\tau}} + \beta(\varphi)\,\mathbf{v}_{\boldsymbol{\tau}} = \mathcal{L}_\varphi\nabla_{\boldsymbol{\tau}}\varphi, & \text{on } \Sigma_T, \\ \partial_t\varphi + \mathbf{v}_{\boldsymbol{\tau}}\cdot\nabla_{\boldsymbol{\tau}}\varphi = -l_0(\varphi)\,\mathcal{L}_\varphi, & \text{on } \Sigma_T, \end{cases} \tag{A.13}$$

where

$$\mathcal{L}_\varphi = \frac{\partial\Phi_s}{\partial\varphi} + \frac{\partial\Phi_b}{\partial\nabla\varphi}\cdot\mathbf{n} - \mathrm{div}_{\boldsymbol{\tau}}\left(\frac{\partial\Phi_s}{\partial\nabla_{\boldsymbol{\tau}}\varphi}\right), \qquad \text{on } \Sigma_T. \tag{A.14}$$

Finally, we make some comments on the above model derivation.

(1) Using (A.1), the expression of $\mathbf{J}_\varphi$ and the incompressibility condition $\nabla\cdot\mathbf{v} = 0$, we infer from the Cahn–Hilliard equation for φ in (A.12) that

$$\partial_t\rho + \mathrm{div}(\rho\mathbf{v} + \mathbf{J}) = 0, \qquad \text{where} \quad \mathbf{J} = \frac{\partial\rho}{\partial\varphi}\mathbf{J}_\varphi.$$

As a consequence, the Navier–Stokes equation for $\mathbf{v}$ in (A.12) can be rewritten as

$$\partial_t(\rho\mathbf{v}) + \mathrm{div}\,(\rho\mathbf{v}\otimes\mathbf{v}) - \mathrm{div}\,(2\nu(\varphi)\,D\mathbf{v}) + \nabla p + \mathrm{div}(\mathbf{v}\otimes\mathbf{J}) = \mu_\varphi\nabla\varphi,$$

which is exactly the same as in (1.1).

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(2) If we choose the viscosity parameter in (A.9) as $\nu(\varphi, D\mathbf{v})$, then non-Newtonian effects, for example, shear thinning or shear thickening, can be included as well.

(3) The interfacial force term $\mu_\varphi \nabla\varphi$ can also be written as

$$\nabla(\Phi_b(\varphi, \nabla\varphi)) - \operatorname{div}\left(\nabla\varphi \otimes \frac{\partial \Phi_b(\varphi, \nabla\varphi)}{\partial \nabla\varphi}\right).$$

Thus, the first term may be regarded as an extra-pressure whereas $\nabla\varphi \otimes \frac{\partial \Phi_b}{\partial \nabla\varphi}$ provides an additional stress tensor contribution which represents interfacial forces.

(3) The uncompensated Young stress $\mathcal{L}_\varphi \nabla_{\boldsymbol{\tau}}\varphi$ on the right-hand side of the generalized Navier boundary condition in (A.13) is simply the manifestation of the fluid–fluid interfacial tension at the solid boundary, whereas the dynamic boundary condition in (A.13) is a consequence of the contact line moving with respect to the solid wall Γ.

(4) If a more general density ρ is desired than a linear dependence in (A.1), the momentum equation of (A.12) must also incorporate an additional source proportional to $(1/2)\, R\mathbf{v}$ (R is given by (1.16)) in order to obtain a local energy dissipation inequality as well as a global energy law for the resulting system. We refer the readers to [4] for further discussions.

Appendix B. Supporting Technical Tools

We report here some technical lemmas that have been used in our analysis. First, we recall the compactness lemma of Aubin–Lions–Simon type (see, for instance, [47] in the case $q > 1$ and [67] when $q = 1$).

Lemma B.1. *Let $X_0 \overset{c}{\hookrightarrow} X_1 \subset X_2$ where X_j are (real) Banach spaces ($j = 1, 2, 3$). Let $1 < p \leqq \infty$, $1 \leqq q \leqq \infty$ and I be a bounded subinterval of $\mathbb{R}$. Then, we have the sets*

$$\left\{\varphi \in L^p(I; X_0) : \partial_t\varphi \in L^q(I; X_2)\right\} \overset{c}{\hookrightarrow} L^p(I; X_1), \quad \text{if } 1 < p < \infty,$$

and

$$\left\{\varphi \in L^p(I; X_0) : \partial_t\varphi \in L^q(I; X_2)\right\} \overset{c}{\hookrightarrow} C(I; X_1), \quad \text{if } p = \infty,\ q > 1.$$

The following result gives a weaker version of the Lebesgue (dominated) convergence theorem (see, for example, [20]):

Lemma B.2. *Let $\mathcal{O}$ be a bounded domain in $\mathbb{R}\times\mathbb{R}^d$ and let a sequence $q_n \in L^p(\mathcal{O})$, $p \in (1, \infty)$, be given. Assume that $\|q_n\|_{L^p(\mathcal{O})} \leqq C$, with $C > 0$ independent of n, $q_n \to q$ almost everywhere on $\mathcal{O}$ and $q \in L^p(\mathcal{O})$. Then as $n \to \infty$, $q_n \rightharpoonup q$ weakly in $L^p(\mathcal{O})$.*

We recall a fundamental result on pointwise multiplication of functions in Sobolev spaces on smooth compact manifolds X with or without boundary (see [50]).

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Lemma B.3. *Let $n_X \geqq 1$ be the dimension of X. Let $s, s_1, s_2 \in \mathbb{R}$ be such that*

$$s_1 + s_2 \geqq 0, \qquad \min(s_1, s_2) \geqq s \qquad \text{and} \qquad s_1 + s_2 - s > \frac{n_X}{2},$$

where the strictness of the last two inequalities can be interchanged if $s \in \mathbb{N}_0$. Then, the pointwise multiplication of functions extends uniquely to a continuous bilinear map

$$W^{s_1,2}(X) \otimes W^{s_2,2}(X) \to W^{s,2}(X).$$

Next, we report a basic result on the regularity of an elliptic boundary value problem for (ϕ, ψ) with $\psi = \mathrm{tr}(\phi)$ (see [52, Lemma A.1]).

Lemma B.4. *Consider the following linear elliptic boundary value problem:*

$$\begin{cases} -\Delta\phi = h_1, & \text{in } \Omega, \\ -\Delta_{\boldsymbol{\tau}}\psi + \partial_{\mathbf{n}}\phi + \zeta\psi = h_2, & \text{on } \Gamma, \end{cases}$$

where $\zeta > 0$ and $(h_1, h_2) \in L^2(\Omega) \times L^2(\Gamma)$. Then the following estimate holds:

$$\|\phi\|_{H^2(\Omega)} + \|\psi\|_{H^2(\Gamma)} \leqq C\left(\|h_1\|_{L^2(\Omega)} + \|h_2\|_{L^2(\Gamma)}\right),$$

for some constant $C > 0$ independent of (ϕ, ψ).

The following lemma provides an easy way to approximate an initial datum (φ_0, ψ_0)
$\in V^1$ by a sequence of smooth functions:

Lemma B.5. *Let $(\varphi_0, \psi_0) \in V^1$ be given. There exists a sequence $\{(\varphi_{0N}, \psi_{0N})\}_{N\in\mathbb{N}}$ $\subset V^2$ such that $(\varphi_{0N}, \psi_{0N}) \to (\varphi_0, \psi_0)$ in the V^1-norm as $N \to \infty$.*

Proof. Let (u, v) be a solution of the (linear) parabolic problem associated with the Wentzell Laplacian A_W, namely,

$$\begin{cases} \partial_t u - \Delta u = 0, & \text{in } Q_T, \\ \partial_t v - \Delta_\Gamma v + \partial_{\mathbf{n}} u + \zeta v = 0, & \text{on } \Sigma_T, \\ (u, v)|_{t=0} = (\varphi_0, \psi_0), & \text{in } \Omega \times \Gamma. \end{cases}$$

Then it holds that

$$(u, v) \in C\left((0, T]; V^2\right) \cap C\left([0, T]; V^1\right).$$

Set $(\varphi_{0N}, \psi_{0N}) := (u(t), v(t))|_{t=\frac{1}{N}}$. We have $(\varphi_{0N}, \psi_{0N}) \in V^2$ and $(\varphi_{0N}, \psi_{0N})$ $\to (\varphi_0, \psi_0)$ in V^1, as $N \to \infty$, by the standard semigroup theory associated with A_W.

The following result is helpful to obtain a (strong) energy inequality (see [2, Lemma 4.3]):

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Lemma B.6. *Let $\mathcal{E} : [0, T) \to [0, \infty)$, $0 < T \leqq \infty$, be a lower semi-continuous function and let $\mathcal{D} : (0, T) \to [0, \infty)$ be an integrable function. Then*

$$\mathcal{E}(0)\eta(0) + \int_0^T \mathcal{E}(t)\eta'(t)dt \geqq \int_0^T \mathcal{D}(t)\eta(t)dt \tag{B.1}$$

holds for all $\eta \in W^{1,1}(0, T)$ with $\eta(T) = 0$ and $\eta \geqq 0$ if and only if

$$\mathcal{E}(t) + \int_s^t \mathcal{D}(\tau)d\tau \leqq \mathcal{E}(s) \tag{B.2}$$

holds for all $s \leqq t < T$ and almost all $0 \leqq s < T$ including $s = 0$.

Finally, we report a result that can be proven in a similar way as to [5, Lemma 5.1].

Lemma B.7. *Let $\mathbf{v}, \tilde{\mathbf{v}} \in \mathbb{H}^1$ and $\rho \in L^\infty(\Omega)$ with $\rho \geqq \rho_0 > 0$ such that*

$$\int_\Omega \rho \mathbf{v} \cdot \boldsymbol{w} dx = \int_\Omega \rho \tilde{\mathbf{v}} \cdot \mathbf{w} dx, \quad \forall\, \mathbf{w} \in \mathbb{C}^\infty_{\mathrm{div}}(\overline{\Omega}).$$

2 *Then it holds that $\mathbf{v} = \tilde{\mathbf{v}}$ almost everywhere in Ω.*

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