Gradient Structures for Flows of Concentrated Suspensions

Dirk Peschka, Marita Thomas, Tobias Ahnert, Andreas Münch, Barbara Wagner

Abstract In this work we investigate a two-phase model for concentrated suspensions. We construct a PDE formulation using a gradient flow structure featuring dissipative coupling between fluid and solid phase as well as different driving forces. Our construction is based on the concept of flow maps that also allows it to account for flows in moving domains with free boundaries. The major difference compared to similar existing approaches is the incorporation of a non-smooth two-homogeneous term to the dissipation potential, which creates a normal pressure even for pure shear flows.

1 Introduction

Suspension flows of solid particles in a viscous liquid are omnipresent in nature and are involved in many technological processes, *e.g.*, in the food, pharmaceutical,

---

Dirk Peschka
Weierstrass Institute Berlin, Mohrenstr. 39, 10117 Berlin, Germany, e-mail: peschka@wias-berlin.de

Marita Thomas
Weierstrass Institute Berlin, Mohrenstr. 39, 10117 Berlin, Germany, e-mail: thomas@wias-berlin.de

Tobias Ahnert
Deloitte Consulting, Hohenzollerndamm 150-151, 14199 Berlin, Germany, e-mail: tahnert@deloitte.de

Andreas Münch
Mathematical Institute, University of Oxford, Andrew Wiles Building, Oxford OX2 6GG, UK e-mail: muench@maths.ox.ac.uk

Barbara Wagner
Weierstrass Institute Berlin, Mohrenstr. 39, 10117 Berlin, Germany, e-mail: Barbara.Wagner@wias-berlin.de

M. Hintermüller, J. F. Rodrigues (eds.), *Topics in Applied Analysis and Optimisation*,
CIM Series in Mathematical Sciences, https://doi.org/10.1007/978-3-030-33116-0_12

printing or oil industries. The fraction of volume occupied by solid particles $0 \leq \phi_s \leq 1$ relative to the combined solid and liquid content, as shown in Figure 1, strongly affects the suspension flow. For very small volume fraction ϕ_s the suspension is called *dilute*, and mutual interaction between particles is neglegible. For increasing volume fraction of the particles the suspension enters a number of flow regimes and rheological behaviours, from shear thinning, to discontinuous shear thickening until it enters the shear *jamming* transition, when a critical volume fraction ϕ_{crit} is reached. Suspensions in this state are called *dense* or *concentrated*. The actual value of ϕ_{crit} depends sensitively on the particle shape, surface and other material properties.

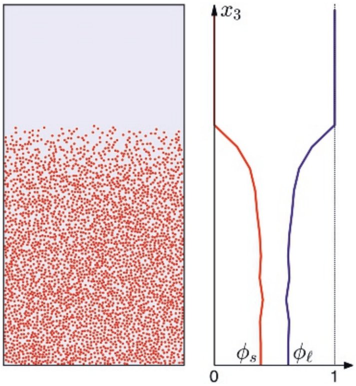

Fig. 1: Discrete solid particle distribution and corresponding volume fractions ϕ_s, ϕ_ℓ. Left: characterstic functions of particles $P : \Omega \to \{0, 1\}$ and Right: volume fractions $\phi_s : \Omega \to [0, 1] \equiv \langle P \rangle$ defined by a suitable average.

Predictive models therefore need to link the interaction of solid particles with the liquid and with other particles on the micro scale with the large-scale description of the dynamics of the liquid and solid phases on the continuum scale. In Figure 2 the numerical simulation of the sedimentation of two-dimensional particles in a viscous liquid is shown. The sedimentation of a particle is certainly influenced by the presence of other particles that create mututal long-ranged interactions due to the fluid flow. On the continuum scale, such a two-phase model works with averaged flow quantities such as averaged velocity $\mathbf{u}$, or effective viscosity μ_{eff} which relates the deviatoric[1] stress τ and the shear rate $\mathbb{D}\mathbf{u} = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^\top)$ via $\tau = 2\mu_{\text{eff}} \operatorname{dev} \mathbb{D}\mathbf{u}$. For dilute suspensions of Newtonian liquids with viscosity μ and spherical particles Einstein [12] derived the effective viscosity law

$$\frac{\mu_{\text{eff}}}{\mu} = 1 + \frac{5}{2}\phi_s. \tag{1.1}$$

[1] The deviator of a tensor/matrix in dimension d is defined as $\operatorname{dev} A = A - d^{-1} \operatorname{tr}(A)\mathbb{I}$ with $\mathbb{I}$ the $d \times d$ unit matrix. It is $\operatorname{tr} \operatorname{dev} A \equiv 0$ by construction. Subsequently we use σ to denote the total (Cauchy) stress, τ for the deviatoric stress, and p for the normal stress/pressure.

However, for many problems suspensions are not dilute but exhibit complex phenomena such as the formation of aggregates, creation of dense sedimentation layers, and shear-induced phase separation into highly concentrated and dilute regions. In fact, for any suspension where the liquid phase evaporates, Einstein's result (1.1) or its extensions [4] will eventually fail.

For many decades a great number of experimental and theoretical studies have been devoted to obtain expressions for an effective viscosity for the regime of concentrated suspensions, such as the Krieger-Dougherty law [21]. It has been observed experimentally that, as the suspension attains a solid-like state, it undergoes a jamming transition and develops further distinct phases [8, 16, 19, 27, 32]. These studies focussed on examining the role of friction and other properties of the particles interacting with each other and the liquid, reflecting how these microscopic properties control large-scale networked patterns. The dramatic increase in research devoted to this topic is rooted in the ground-breaking experimental study by Cassar et al. [7], where it was found that a dense suspension on an inclined plane sheared at a rate $2|\mathbb{D}\mathbf{u}|$ under a confining pressure p_c can be characterized by a single dimensionless control parameter, the viscous number

$$I_v = \frac{2\mu|\mathbb{D}\mathbf{u}|}{p_c}. \tag{1.2}$$

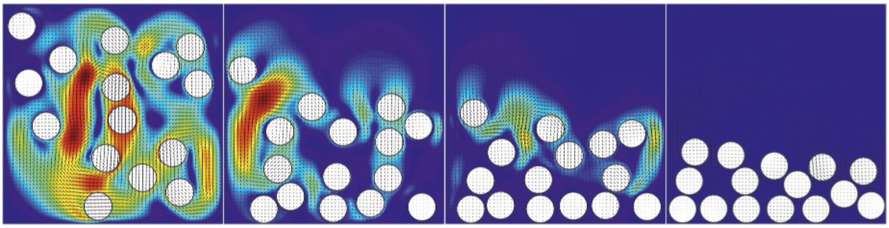

Fig. 2: Particulate flow with gravity in $\Omega \subset \mathbb{R}^2$ showing the sedimentation in a suspension with time advancing from left to right. The particle indictor function $P : \Omega \to \{0, 1\}$ is shown using white discs, the shading indicates the magnitude of the velocity field, shown using vectors.

This result was taken up by Boyer et al. [5], where a new constitutive friction law combining the rheology for non-Brownian suspensions and granular flows has been proposed, and for the first time offers to quantitatively capture the jamming transition. In Ahnert et al. [1], this new constitutive friction law was incorporated in the derivation of a new two-phase model for non-homogeneous shear flows and studied for simple shear flows such as plane Couette and Poiseuille flow. One key feature of these suspension models is the appearance of the normal or contact pressures p_c, with their role for particle migration discussed by Morris & Boulay [24].

Beyond simple effective models, predictive models on the length scale of these applications need to combine the interactions of the liquid and solid particles among each other on the microscale with a description of the dynamics of the liquid and solid phase on the continuum scale. This requires to incorporate phenomena such as transport of volume and mass with the balances of momenta and forces. The solid and liquid phase, i.e., their volume fractions ϕ_s and $\phi_\ell = 1 - \phi_s$, are transported by individual velocities $\mathbf{u}_s$ and $\mathbf{u}_\ell$. The velocities themselves obey the momentum balances of solid and liquid phase and are dissipative due to the presence of viscosity. Similar phenomena are known in the literature for classical mixture models.

To obtain further insight into the mathematical structure of this model we discuss in this article two-phase flow models from an energetic point of view and obtain that the general mathematical structure behind is of gradient-flow type. Hence, the evolution of the model system is characterized in terms of an energy functional and a dissipation potential. In particular, we will use the property that the model for the different regimes, from dilute to highly concentrated states, have a common general mathematical structure of variational type. In the long run, this will allow it to pursue the limit passage using variational convergence methods, and thus to carry out the transition from a dilute to a concentrated suspension as a rigorous scaling limit.

The focus of this work is to construct a class of thermodynamically and mechanically consistent models that support normal pressures using the framework of variational modelling. We present a method to construct suspension models with free boundaries and provide the underlying construction for gravity driven and surface-tension driven flows. Examples of such flows are given in applications such as in Murisic et al. [26].

2 Model for a concentrated suspension

We briefly summarise the dense suspension model that was derived in Ahnert et al. [1], by averaging the microscopic formulation of the flow with a liquid and a particulate solid phase along the lines of Drew [9] and Drew & Passman [10], in combination with a constitutive law for the solid phase stress-strain rate relation based on the results of the experiments by Boyer et al. [5] and a Kozeny-Carman relation for the interphase drag, see for example Brennen [6]. We assumed that the suspension consists of monodisperse, spherical, non-Brownian particles. It is also assumed that the mass densities of the solid ρ_s and liquid phase ρ_ℓ are constant. The equations are stated in non-dimensional variables as explained in detail in [1]; here we only give a brief summary of the scalings and the resulting equations. We use a velocity scale U, a length scale L, a time scale L/U and a viscous scale $\mu_\ell U/\rho_\ell$ for the pressure and stress field, where μ_ℓ is the liquid phase viscosity. The variables ϕ_s, $\mathbf{u}_s$, τ_s and p_s denote the volume fraction, velocity, deviatoric stress and normal stress for the solid phase, respectively, and analogously ϕ_ℓ, $\mathbf{u}_\ell$, τ_ℓ and p_ℓ for the liquid phase; t is the time. (The index ℓ is ommitted from the liquid pressure to be consistent with notation for the Lagrange multiplier in subsequent sections.) The bars $|\cdot|$ represent the componentwise Euclidean norm of a vector or tensor. Without inertia, the mass conservation and momentum balance equations for the two phases are

$$\partial_t \phi_\ell + \nabla \cdot (\phi_\ell \mathbf{u}_\ell) = 0, \tag{2.1a}$$
$$\partial_t \phi_s + \nabla \cdot (\phi_s \mathbf{u}_s) = 0, \tag{2.1b}$$
$$-\nabla \cdot \sigma_\ell + M_d + \phi_\ell \nabla \pi = 0, \tag{2.1c}$$
$$-\nabla \cdot \sigma_s - M_d + \phi_s \nabla \pi = 0, \tag{2.1d}$$

where the total stresses in liquid and solid phase are

$$\sigma_\ell(\mathbf{u}_\ell) = -p_\ell(\mathbf{u}_\ell)\mathbb{I} + \tau_\ell(\mathbf{u}_\ell), \tag{2.1e}$$
$$\sigma_s(\mathbf{u}_s) = -\big(p_c(\mathbf{u}_s) + p_s(\mathbf{u}_s)\big)\mathbb{I} + \tau_s(\mathbf{u}_s). \tag{2.1f}$$

The Lagrange multiplier π takes care of the constraint $\mathrm{div}_x(\phi_s \mathbf{u}_s + \phi_\ell \mathbf{u}_\ell) = 0$, which results from the condition $\phi_s + \phi_\ell = 0$ upon differentiation with respect to time using the transport equations. The drag M_d is given by the non-dimensional form of the Kozeny-Carman relation

$$M_d = \mathrm{Da}\,\frac{\phi_s^2}{\phi_\ell}(\mathbf{u}_\ell - \mathbf{u}_s). \tag{2.2}$$

The Darcy number which appears here is $\mathrm{Da} = L^2/K_p^2$, where K_p is proportional to the square of the particle diameter, so that Da is typically large. Next we specify the constitutive equations for the rheology of the liquid and the solid phase. For the liquid phase in three space dimensions, i.e., for $d = 3$, we have

$$p_\ell = -\frac{2}{3}\phi_\ell\,\mathrm{div}_x(\mathbf{u}_\ell), \qquad \tau_\ell = 2\phi_\ell\,\mathrm{dev}\,\mathbb{D}\mathbf{u}_\ell, \tag{2.3}$$

with $\mathbb{D}\mathbf{u}_\ell = \left(\nabla\mathbf{u}_\ell + \nabla\mathbf{u}_\ell^T\right)/2$ the shear rate. For the solid phase, if $|\mathbb{D}\mathbf{u}_s| > 0$, then

$$p_s = -\frac{2}{3}\phi_s\eta_s(\phi_s)\,\mathrm{div}_x\,\mathbf{u}_s, \qquad \tau_s = 2\phi_s\eta_s(\phi_s)\,\mathrm{dev}\,\mathbb{D}\mathbf{u}_s, \tag{2.4a}$$

with $\mathrm{dev}\,A = A - \frac{1}{3}\,\mathrm{tr}A$ the deviator of a matrix $A \in \mathbb{R}^{3\times 3}$; additionally there also acts a contact pressure given by

$$p_c = 2\phi_s\eta_n(\phi_s)|\mathbb{D}\mathbf{u}_s|. \tag{2.4b}$$

For $i = s, \ell$ note that $p_i = 0$ for divergence-free flows $\mathrm{div}_x\,\mathbf{u}_i = 0$, whereas p_c only vanishes when $\mathbb{D}\mathbf{u}_s$ does so. The constitutive material laws in the above definitions are

$$\eta_s(\phi_s) = 1 + \frac{5}{2}\frac{\phi_{\text{crit}}}{\phi_{\text{crit}} - \phi_s} + \mu_c(\phi_s)\frac{\phi_s}{(\phi_{\text{crit}} - \phi_s)^2}, \tag{2.4c}$$

$$\mu_c(\phi_s) = \mu_1 + \frac{\mu_2 - \mu_1}{1 + I_0\phi_s^2(\phi_{\text{crit}} - \phi_s)^{-2}}, \tag{2.4d}$$

$$\eta_n(\phi_s) = \left(\frac{\phi_s}{\phi_{\text{crit}} - \phi_s}\right)^2, \tag{2.4e}$$

with the non-dimensional parameters, $\mu_2 \geq \mu_1, I_0$, and the maximum volume fraction ϕ_{crit} for a random close packing. Instead, if $\mathbb{D}\mathbf{u}_s = 0$, we require

$$\phi_s = \phi_{\text{crit}}, \tag{2.4f}$$

and

$$|\sigma_s| \leq \mu_1 p_c. \tag{2.4g}$$

A typical value for the maximum random packing fraction is $\phi_{\text{crit}} = 0.63$. The values suggested in Boyer et al. [5] for the other parameters are $\mu_2 = 0.7$, and $I_0 = 0.005$, but these lead to a problem with ill-posedness even for plane Poiseuille flow [1].

The constitutive law (2.4) has the following implications: Given a fixed, positive finite contact pressure p_c, if the shear rate $\mathbb{D}\mathbf{u}_s$ tends to zero, then $\eta_n = p_c/(2\phi_s|\mathbb{D}\mathbf{u}_s|) \to \infty$ and thus $(\phi_{\text{crit}} - \phi_s) \to 0$. Since η_s has the same singular dependence on $\phi_{\text{crit}} - \phi_s$, it tends to infinity at the same rate and, therefore, $|\sigma_s|$ tends to a finite positive value, $\mu_1 p_c/\phi_s$, which gives rise to the yield stress in (2.4g). Across a yield surface, we require that ϕ_s, $\mathbf{u}_\ell$, $\mathbf{u}_s$, $|\mathbb{D}\mathbf{u}_s|$ and the projection of $-p_\ell\mathbb{I} + \tau_\ell$ and $-(p_s + p_c)\mathbb{I} + \tau_s$ onto the surface normal are continuous. While the suspension model above is stated for simplicity without any additional external forces, the later gradient flow construction will contain the full model with forces arising due to certain bulk or surface energies.

3 Gradient flow for two-phase flows of concentrated suspensions

Beyond flows of purely viscous liquids, the discussion of the proper mechanical statement of models for multi-phase flows has been studied extensively in the past, *e.g.*, [9, 10, 18, 20]. A major challenge from the modelling point of view is the construction of models that are mathematically, thermodynamically and mechanically meaningful. We here construct a class of models using a *variational approach* based on the energy and dissipation functionals related to the processes. In this way, we will deduce one possible model to describe flows of two-phase mixtures with free, evolving boundaries and provide the underlying construction for gravity-driven and surface-tension driven flows.

First variational descriptions of fluid flows are due to Helmholtz [15] and Rayleigh [31]. A general framework for the thermodynamic description of fluids has been layed out by Öttinger & Grmela [14, 28]. For the special construction of Euler flows using Poisson structures has been reviewed, for instance, by Morrison [25]. Peletier [29] gave a well-structured overview of systems which can be casted as gradient flows. For an extensive overview of different models for complex fluids and flow maps we refer to the recent review by Giga et al. [13]. It has to be stressed that the afore mentioned contributions consider the flow in fixed domains with fixed boundaries. In fact, our approach can be seen as a generalization of the one presented in [13] for single-phase fluid flow in a fixed domain to the problem of two-phase flows on evolving domains.

In the following we focus on the formal description of free boundary multi-phase flows on moving domains in terms of generalized gradient flows. This concept has been discussed e.g. by Mielke [22] in an abstract framework and formally applied to models arising in many different applications. Following [22], such a description is based the specification of a triple $(\mathbf{V}, \mathcal{R}, \mathcal{E})$ consisting of the (Banach) space of velocities, a dissipation potential $\mathcal{R} : \mathbf{Q} \times \mathbf{V} \to [0, \infty]$, and an energy functional $\mathcal{E} : \mathbf{Q} \to \mathbb{R}$ defined on the state space $\mathbf{Q}$. Elements of the state space are denoted by $q \in \mathbf{Q}$ and their corresponding velocities by $\dot{q} \in \mathbf{V}$. For all states $q \in \mathbf{Q}$ it is required that $\mathcal{R}(q; \cdot) : \mathbf{V} \to [0, \infty]$ is convex and that $\mathcal{R}(q; \dot{q} = 0) = 0$. With $\mathbf{V}^*$ we denote the dual space of $\mathbf{V}$ and define for fixed $q \in \mathbf{Q}$ the dual dissipation functional $\mathcal{R}^*(q, \cdot) : \mathbf{V}^* \to [0, \infty]$ as the convex conjugate of $\mathcal{R}(q; \cdot)$, i.e., for all $v^* \in \mathbf{V}^*$ it is $\mathcal{R}^*(q, v^*) := \sup_{v \in \mathbf{V}} \left(\langle v^*, v \rangle_{\mathbf{V}} - \mathcal{R}(q, v) \right)$. As in [22] we speak here of a generalized gradient flow as we neither require $\mathcal{R}$ to be quadratic nor classically differentiable. In this generalized setting it can be shown, cf. e.g. [22, 23], by exploiting the convexity of the functionals $\mathcal{R}(q, \cdot)$ and $\mathcal{R}^*(q, \cdot)$ that a solution $q : [0, T] \to \mathbf{Q}$ of $(\mathbf{V}, \mathcal{R}, \mathcal{E})$ is characterized by the following three equivalent problem formulations:

$$
\begin{aligned}
& \dot{q}(t) \in \partial \mathcal{R}^*(q(t), -\mathrm{D}_q \mathcal{E}(q(t))) && \text{in } \mathbf{V}, && (3.1a)\\
\Leftrightarrow \quad & -\mathrm{D}_q \mathcal{E}(q(t)) \in \partial \mathcal{R}(q(t), \dot{q}(t)) && \text{in } \mathbf{V}^*, && (3.1b)\\
\Leftrightarrow \quad & \langle -\mathrm{D}_q \mathcal{E}(q(t)), \dot{q}(t) \rangle_{\mathbf{V}} = \mathcal{R}(q(t), \dot{q}(t)) + \mathcal{R}^*(q(t), -\mathrm{D}_q \mathcal{E}(q(t))), && && (3.1c)
\end{aligned}
$$

where $\partial(\cdot)$ denotes the subdifferential of a convex functional with respect to $\dot{q}$ and $\mathrm{D}\mathcal{E}(q)$ the Fréchet-derivative of $\mathcal{E}$.

Since the Young-Fenchel inequality for convex functionals and their conjugate always ensures $\langle -\mathrm{D}_q \mathcal{E}(q), \dot{q} \rangle_{\mathbf{V}} \le \mathcal{R}(q, \dot{q}) + \mathcal{R}^*(q, -\mathrm{D}_q \mathcal{E}(q))$ one can infer from (3.1c) that the time-derivative $\dot{q}$ of a solution q of (3.1) also satisfies

$$
\dot{q} \in \operatorname{argmin}_{\dot{q} \in \mathbf{V}} \left(\langle \mathrm{D}_q \mathcal{E}(q), \dot{q} \rangle_{\mathbf{V}} + \mathcal{R}(q, \dot{q}) \right), \qquad (3.1d)
$$

since $\mathcal{R}^*(q(t), -\mathrm{D}_q \mathcal{E}(q(t)))$ is independent of $\dot{q}$.

Indeed, the setting of generalized gradient flows based on convex potentials with the formulation (3.1) provides a generalization of classical gradient flows characterized by quadratic potentials. For a given self-adjoint linear operator $G(q) : \mathbf{V} \to \mathbf{V}^*$ and quadratic functionals $\mathcal{R}(q, \dot{q}) = \frac{1}{2} \langle G(q) \dot{q}, \dot{q} \rangle$ a solution $q(t)$ of the gradient flow is given by a curve $q : [0, T] \to \mathbf{Q}$ satisfying (3.1b), which reads in this smooth, quadratic context as

$$\dot{q}(t) = -\nabla_{\mathcal{R}}\mathcal{E}\big(q(t)\big). \tag{3.1e}$$

where the gradient $v = \nabla_{\mathcal{R}}\mathcal{E}(q) \in \mathbf{V}$ of $\mathcal{E}$ with respect to the metric induced by $\mathcal{R}$ is defined by $\langle G(q)^* v, \dot{\tilde{q}}\rangle = \langle G(q)^* \mathrm{D}_q\mathcal{E}(q), \dot{\tilde{q}}\rangle$ for all $\dot{\tilde{q}} \in \mathbf{V}$ and $G(q) = G(q)^*$.

Formulation (3.1) provides the abstract framework that we are going to use in order to deduce two-phase suspension models on moving domains. More precisely, in this section we will show that, under suitable smoothness assumptions on the functions involved, flow models for suspensions as discussed in the previous Section 2 indeed arise as generalized gradient flows $(\mathbf{V}, \mathcal{R}, \mathcal{E})$ in the form (3.1b). Given a suitable triple $(\mathbf{V}, \mathcal{R}, \mathcal{E})$ we will rigorously derive a weak formulation of the corresponding PDE system (3.1b). At this point our presentation will stay on a formal level, as we will not address the existence and regularity of solutions for the resulting problem. Under further smoothness assumptions we will then formally deduce a pointwise formulation of the associated Cauchy problem and compare our resulting system with the one presented in Section 2. Indeed, we shall see that a dissipation potential suited to produce a critical pressure of 1-homogeneous nature is not of the standard smooth, quadratic nature.

3.1 Notation and states

We consider the motion of a liquid continuous phase (index ℓ) mixed with a solid dispersed phase of non-Brownian particles (index s) phase occupying at each time $t \in [0, T]$ a bounded set $\Omega(t) \subset \mathbb{R}^d$ where $d \in \mathbb{N}$. At the initial time $t = 0$ this subdomain is denoted by $\bar{\Omega} = \Omega(0)$. For each point in space $x \in \Omega(t)$ the state of the suspension is characterized by volume fractions $0 \le \phi_s(t,x), \phi_\ell(t,x) \le 1$ such that we have $\phi_s(t,x) + \phi_\ell(t,x) = 1$ pointwise. In the following we define the structures needed to model the evolution of ϕ_i and $\Omega(t)$ using a gradient flow structure. One key idea in this construction is the consistent use of *flow maps* as elements of an abstract state space.

Definition 1 (Evolution of shapes with flow maps) Let $\chi(t,\cdot) : \bar{\Omega} \to \Omega(t)$ a family of diffeomorphisms that map from $\bar{\Omega} \subset \mathbb{R}^d$ to $\Omega(t) \subset \mathbb{R}^d$ using

$$\Omega(t) = \chi(t, \bar{\Omega}) \equiv \{x \in \mathbb{R}^d : \exists X \in \bar{\Omega} \ s.t. \ x = \chi(t, X)\}. \tag{3.2}$$

The small letter x will always denote coordinates in $\Omega(t)$, whereas the capital letter X denotes coordinates in the reference configuration $X \in \bar{\Omega}$. We define the associated velocity $\mathbf{u}(t,\cdot) : \Omega(t) \to \mathbb{R}^d$ with

$$\mathbf{u}(t,x) = \big(\partial_t \chi\big)(t, \chi^{-1}(t,x)). \tag{3.3}$$

We call $\chi(t,\cdot)$ the *flow map* associated to the motion of $\Omega(t)$ and $\mathbf{u}(t,\cdot)$ the corresponding velocity vector field. Initial data are chosen such that $\chi(t = 0, X) = X$ and $\bar{\Omega} = \Omega(0)$. With the notation $F_\chi = \nabla_X \chi$ we indicate the gradient of the transformation and assume for its Jacobian determinant that $\det F_\chi > 0$. On the other hand, for

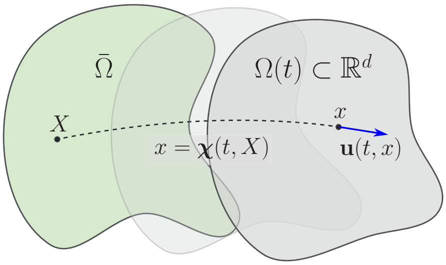

Fig. 3: Flow map $\boldsymbol{\chi}(t,\cdot) : \bar{\Omega} \to \Omega(t)$ mapping a point $X \in \bar{\Omega} \subset \mathbb{R}^d$ from the reference domain $\bar{\Omega}$ (green shaded) to a point in the mapped configuration $\Omega(t)$ (gray shaded). When considering the trajectory $x(t) = \boldsymbol{\chi}(t, X)$ (dashed line) for any given X, then $\mathbf{u} = \dot{x}(t)$ is the associated velocity (arrow) and $\mathbf{u}(t, x)$ the corresponding flow field.

given flow field $\mathbf{u}$ we have an associated ODE-Cauchy problem:

$$\partial_t \boldsymbol{\chi}(t, X) = \mathbf{u}(t, \boldsymbol{\chi}(t, X)) \qquad \text{for all } X \in \bar{\Omega} \text{ and } t \in [0, T], \tag{3.4a}$$

$$\boldsymbol{\chi}(0, X) = X \qquad \text{for all } X \in \bar{\Omega}. \tag{3.4b}$$

Note that (3.4) is the *kinematic condition* for the domain motion.

In the presence of two phases, each phase is characterized by its own flow map $\boldsymbol{\chi}_i : [0, T] \times \bar{\Omega} \to \Omega(t) \subset \mathbb{R}^d$ with $i \in \{s, \ell\}$ for solid and liquid phase. Correspondingly we use $\mathbf{u}_i$ and F_i to indicate the corresponding velocities and Jacobians. With this notation we further require the flow maps to satisfy the following assumptions: Multiple flow maps are defined on the same domain

$$\Omega(t) = \boldsymbol{\chi}_s(t, \bar{\Omega}) = \boldsymbol{\chi}_\ell(t, \bar{\Omega}), \tag{3.5}$$

which of course does not imply that the flow maps are equal. Furthermore we have the following assumptions on $\mathbf{u}_i$ and $\boldsymbol{\chi}_i$ for $i \in \{s, \ell\}$ for all $t \in [0, T]$:

- $\Omega(t)$ and $\bar{\Omega}$ bounded and sufficiently smooth, (3.6a)
- $\boldsymbol{\chi}_i(t,\cdot) : \bar{\Omega} \to \Omega(t)$ is a smooth diffeomorphism, (3.6b)
- $\det F_i(t,\cdot) > 0$, where $F_i(t, X) = \nabla_X \boldsymbol{\chi}_i(t, X)$, (3.6c)
- $\mathbf{u}_s(t,\cdot) = \mathbf{u}_\ell(t,\cdot)$ on $\partial\Omega(t)$. (3.6d)

Note that for the gradient structure equality of tangential velocities on the boundary would suffice to ensure (3.5), but we require the slightly stronger condition (3.6d).

At each time $t \in [0, T]$ and each $x \in \Omega(t)$, the fraction of volume occupied by liquid and solid phase is characterized by the two phase indicators $\phi_i(t, x), i \in \{s, \ell\}$. Since ϕ_i represent volume fractions, they must satisfy

$$\phi_s(t, x), \phi_\ell(t, x) \in [0, 1] \quad \text{for all } t \in [0, T] \text{ and all } x \in \Omega(t) \tag{3.7a}$$

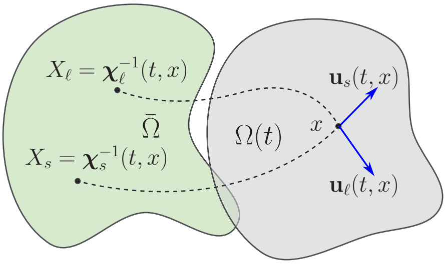

Fig. 4: Flow maps $\chi_i(t,\cdot)$ for solid $i = s$ phase and liquid $i = \ell$ phase mapping a point $X \in \bar{\Omega} \subset \mathbb{R}^d$ from the reference domain $\bar{\Omega}$ (green shaded) to a point in the mapped configuration $\Omega(t)$ (gray shaded). When considering the trajectories $x_i(t) = \chi_i(t,X)$ (dashed lines) for any given X and $i \in \{s,\ell\}$, then $\mathbf{u}_i = \dot{x}_i(t)$ are the associated velocities (arrow) and $\mathbf{u}_i(t,x)$ the corresponding flow field. At time t the trajectories meet at the same point x, when they started at $X_i = \chi_i^{-1}(t,x)$.

and fill the volume such that

$$\phi_s(t,x) + \phi_\ell(t,x) = 1 \quad \text{for all } t \in [0,T] \text{ and all } x \in \Omega(t) \tag{3.7b}$$

The evolution of the densities is defined via a local conservation law for the two volume fractions. We assume that the given initial volume fractions $\phi_i(t = 0, X) = \bar{\phi}_i(X) \in [0,1]$ and that the flow maps $\chi_i(t,\cdot) : \bar{\Omega} \to \Omega(t)$ as well as their velocities $\mathbf{u}_i(t,\cdot) : \Omega(t) \to \mathbb{R}^d$ are sufficiently smooth for $i \in \{s,\ell\}$. For arbitrary $\bar{\omega} \subset \bar{\Omega}$ let $\omega_i(t) = \chi_i(t,\bar{\omega}) \subset \Omega(t)$. In the absence of reaction or diffusion processes we require the volume fraction $\phi_i(t,\cdot) : \Omega(t) \to \mathbb{R}$ to satisfy the *integral form of volume conservation* stated as

$$\int_{\omega(t)} \phi_i(t,x)\,\mathrm{d}x = \int_{\bar{\omega}} \bar{\phi}_i(X)\,\mathrm{d}X. \tag{3.8a}$$

Differentiating (3.8a) in time and using the Reynolds transport theorem, given the smoothness of all quantities involved, shows the equivalent *differential form of volume conservation*: For given $t \in [0,T]$ and any $x \in \Omega(t)$ the density $\phi_i(t,x)$ satisfies the (Cauchy problem for the) transport equation

$$\begin{aligned} &\partial_t \phi_i(t,x) + \mathrm{div}_x\big(\phi_i(t,x)\mathbf{u}_i(t,x)\big) = 0 \quad \text{in } \Omega(t), \\ &\phi_i(0,X) = \bar{\phi}_i(X) \quad \text{in } \bar{\Omega}, \end{aligned} \tag{3.8b}$$

with given, sufficiently smooth initial data $\bar{\phi}_i$, which also have to satisfy the volume constraints, i.e., we claim that

- $0 \le \bar{\phi}_i \le 1 \quad$ for all $X \in \bar{\Omega}$, (3.9a)
- $\bar{\phi}_s + \bar{\phi}_\ell = 1 \quad$ for all $X \in \bar{\Omega}$. (3.9b)

The following lemma summarizes a few immediate consequences of the preceeding definitions, constraints, and assumptions. Moreover, Statement 4. below justifies why we can subsequently work with the divergence contraint (3.10) for the average velocity, cf. the definition of the dissipation potential (3.17), in order to equivalently guarantee the volume constraint (3.7b) for the phase indicators.

Lemma 3.1 *Let $i \in \{s, \ell\}$ and let all the quantities $\chi_i, \phi_i, \mathbf{u}_i, \bar{\phi}_i$ be sufficiently smooth.*

1. *Assume the densities ϕ_i fill the volume (3.7b). Then at each time $t \in [0, T]$ the average velocity defined as $\mathbf{u} = \phi_s \mathbf{u}_s + \phi_\ell \mathbf{u}_\ell$ satisfies the following divergence constraint*

$$\operatorname{div}_x \mathbf{u}(t, x) = 0, \qquad \text{for all } x \in \Omega(t). \tag{3.10}$$

2. *Let the sufficiently smooth flow map also satisfy the positivity assumption (3.6c), i.e.,* $\det F_i > 0$*. Then, the transport problem (3.8) for the volume fraction ϕ_i is equivalent to the following explicit representation for any given $t \in [0, T]$:*

$$\phi_i\big(t, \chi_i(t, X)\big) = \big(\det\, F_i(t, X)\big)^{-1} \bar{\phi}_i(X), \qquad \text{for each } X \in \bar{\Omega}. \tag{3.11}$$

3. *Let the transport problem (3.8) as well as the volume constraint (3.7b) be satisfied. Then the two phase volumes are conserved, i.e.,*

$$V_i(t) = \int_{\Omega(t)} \phi_i(t, x)\, \mathrm{d}x = V_i(0), \qquad \text{and} \qquad |\Omega(t)| = V_s + V_\ell = |\bar{\Omega}|. \tag{3.12}$$

4. *Let the transport problem (3.8) be satisfied. Then, the following equivalence holds true for the volume constraint on the phase indicator:*

$$\left\{ \begin{array}{l} \text{(3.9b) for } \bar{\phi}_s, \bar{\phi}_\ell \text{ at initial time} \\ \text{\& divergence constraint (3.10)} \end{array} \right\} \Leftrightarrow \left\{ \text{(3.7b) for } \phi_s, \phi_\ell \text{ at any } t \in [0, T] \right\} \tag{3.13}$$

5. *Assume that $\bar{\phi}_i$ satisfies the convex constraint (3.9a) at initial time, that the transport relation (3.8) as well as volume constraint (3.9b) and divergence constraint (3.10) hold true. Then the convex constraint (3.7a) holds true also for $\phi_i(t, \cdot)$ in $\Omega(t)$ for any $t \in [0, T]$.*

Proof **To 1.:** Since we assumed $\phi_s(t, x) + \phi_\ell(t, x) = 1$ for any $x \in \Omega(t)$ we readily conclude $\partial_t(\phi_s + \phi_\ell) = 0 = \operatorname{div}_x(\phi_s \mathbf{u}_s + \phi_\ell \mathbf{u}_\ell)$.
To 2.: Using change of variables $X = \chi_i^{-1}(t, x)$ and volume conservation (3.8) we find for all $t \in [0, T]$, arbitrary $\bar{\omega} \subset \bar{\Omega}$ and $\omega(t) = \chi_i(t, \bar{\omega})$ that

$$\int_{\bar{\omega}} \bar{\phi}_i(X)\, \mathrm{d}X = \int_{\omega(t)} \phi_i(t, x)\, \mathrm{d}x = \int_{\bar{\omega}} \phi_i(t, \chi_i(t, X)) \det F_i(t, X)\, \mathrm{d}X\,.$$

The assertion follows due to the smoothness of ϕ_i and the positivity of $\det F_i$.
To 3.: This is a direct consequence of 1. and $\phi_s + \phi_\ell = 1$.

To 4.: Clearly, condition (3.7b) includes (3.9b) initial time. The divergence constraint again follows from (3.7b) and (3.8) along the lines of Item 1.. Hence, '$\Leftarrow$' in (3.13). To find also '$\Rightarrow$' we argue as follows: Transport problem (3.8) together with (3.10) implies $\partial_t(\phi_s + \phi_\ell) = 0$ in $[0,T] \times \Omega(t)$. Hence $\phi_s(t,x) + \phi_\ell(t,x) = c(x) = \phi_s(0,X) + \phi_\ell(0,X) = 1$, which is (3.7b) at any $t \in [0,T]$.

To 5.: The above argument implies $\phi_i \le 1$, if it is possible to show that $\phi_i \ge 0$. Indeed, the latter follows from (3.8) thanks to its equivalence to the representation (3.11). By the positivity of the determinant (3.6c) and the constraint (3.9a) satisfied by the initial data we may thus conclude that $\phi_i \ge 0$. □

Here we point out the crucial observation that the evolution of ϕ_i is not independent but rather defined using the flow maps χ_i. However, when considering functional depending on ϕ_i we need to be able to compute its variations. For this we recall the simple identity for change of variables for volume integrals.

Theorem 3.1 (Change of variables in volumes) *Let* $\chi : (t,\cdot)\bar\Omega \to \Omega$ *a flow map from* $\bar\Omega \subset \mathbb{R}^d$ *to* $\Omega(t) \subset \mathbb{R}^d$ *and let* $\phi(t,\chi(t,X)) = (\det F_\chi)^{-1}\bar\phi(X)$ *and* $f(x,\phi)$ *given.*

$$\int_{\chi(t,\bar\Omega)} f(x,\phi)\,\mathrm{d}x = \int_{\bar\Omega} f\big(\chi(t,X),(\det F_\chi(t,X))^{-1}\bar\phi(X)\big)\,\det F_\chi(t,X)\,\mathrm{d}X.$$

For instance using $f(x,\phi_i) = \phi_i$ and $\chi = \chi_i$ shows that conservation of volume holds by construction since

$$\int_{\chi_i(t,\bar\Omega)} \phi_i(t,x)\,\mathrm{d}x = \int_{\bar\Omega} \bar\phi_i(X)\,\mathrm{d}X = V_i.$$

3.2 The triple $(\mathbf{V},\mathcal{R},\mathcal{E})$ for flows of concentrated suspensions

In view of the discussion in Section 3.1 we denote in the following the vector of states by $q := (\chi_s,\chi_\ell) \in \mathbf{Q}$ and its associated vector of velocities by $\dot q := (\mathbf{u}_s,\mathbf{u}_\ell) \in \mathbf{V}$. Hereby, we will use the spaces

$$\mathbf{X} := \{\chi \in H^1(\bar\Omega;\mathbb{R}^d),\ \chi = \mathrm{id}_{\bar\Omega} \text{ on } \partial\bar\Omega\backslash\bar\Gamma\}, \tag{3.14a}$$
$$\mathbf{Q} := \{(\chi_s,\chi_\ell) \in \mathbf{X}\times\mathbf{X},\ \chi_s = \chi_\ell \text{ on } \bar\Gamma\}, \tag{3.14b}$$

as the state space for the flow maps defined on the reference configuration $\bar\Omega$ and

$$\mathbf{V} := \left\{(\tilde{\mathbf{u}}_s,\tilde{\mathbf{u}}_\ell) \in H^1(\Omega(t);\mathbb{R}^d\times\mathbb{R}^d),\ \begin{array}{ll}\tilde{\mathbf{u}}_s = \tilde{\mathbf{u}}_\ell & \text{on } \Gamma(t)\\ \tilde{\mathbf{u}}_s = \tilde{\mathbf{u}}_\ell = 0 & \text{on } \partial\Omega(t)\backslash\Gamma(t)\end{array}\right\}, \tag{3.15}$$

as the function space for the velocities defined on the current configuration $\Omega(t)$ for all $t \in [0,T]$. Note that above we introduced a part of the boundary $\partial\bar\Omega \setminus \bar\Gamma$, on which the shape of the domain is fixed corresponding to a no-slip boundary condition. Moreover we stress that the upcoming definitions of functionals will always implicitely depend on a vector of given data $(\bar{\phi}_s, \bar{\phi}_\ell, \bar{\Omega})$, which consists of the reference configuration $\bar{\Omega} \subset \mathbb{R}^d$, and of the reference densities $\bar{\phi}_s, \bar{\phi}_\ell$ of solid and fluid phase.

Further using the notation from Definition 1 we consider an energy functional $\mathcal{E} : \mathbf{Q} \to [0,\infty]$ where

$$\mathcal{E}(q) := \mathcal{E}_{\text{bulk}}(q) + \mathcal{E}_{\text{surf}}(q) \quad \text{with}$$

$$\mathcal{E}_{\text{bulk}}(q) := \begin{cases} \int_{\Omega(t)} E(x,\phi_s)\,\mathrm{d}x & \text{if } \phi_i(t,x) = \frac{\bar{\phi}_i(t,X)}{\det F_i(t,X)}, \\ \infty & \text{otherwise,} \end{cases} \tag{3.16a}$$

$$\text{where } E(x,\phi_s) := g x_d(\phi_s\rho_s + (1-\phi_s)\rho_\ell), \quad \text{and} \tag{3.16b}$$

$$\mathcal{E}_{\text{surf}}(q) := \begin{cases} \int_{\Gamma(t)} \vartheta\,\mathrm{d}\mathcal{H}^{d-1} & \text{if } \phi_i(t,x) = \frac{\bar{\phi}_i(t,X)}{\det F_i(t,X)}, \\ \infty & \text{otherwise.} \end{cases} \tag{3.16c}$$

In (3.16b) the constant g denotes the gravity constant, x_d is the dth component of the space variable $x \in \Omega(t) \subset \mathbb{R}^d$ in the current configuration $\Omega(t)$, and ρ_s, ρ_ℓ denote the mass densities of the solid and the fluid phase, respectively. Moreover, in (3.16c), the parameter ϑ denotes the surface tension and $\mathcal{H}^{d-1}$ is the $(d-1)$-dimensional Hausdorff measure.

In addition, we also introduce the dissipation potential $\mathcal{R} : \mathbf{Q} \times \mathbf{V} \to [0,\infty]$ as

$$\mathcal{R}(q;\dot{\tilde{q}}) := \int_{\Omega(t)} R(\phi_s,\phi_\ell;\tilde{\mathbf{u}}_s,\tilde{\mathbf{u}}_\ell,\tilde{e}_s,\tilde{e}_\ell)\,\mathrm{d}x + \mathcal{I}_{\mathbf{K}(q)}(\tilde{\mathbf{u}}_s,\tilde{\mathbf{u}}_\ell), \tag{3.17a}$$

where we used the indicator functional $\mathcal{I}_{\mathbf{K}(q)}$ and the constraint set $\mathbf{K}(q)$ defined as

$$\mathcal{I}_{\mathbf{K}(q)}(\tilde{\mathbf{u}}_s,\tilde{\mathbf{u}}_\ell) := \begin{cases} 0 & \text{if } (\tilde{\mathbf{u}}_s,\tilde{\mathbf{u}}_\ell) \in \mathbf{K}(q), \\ \infty & \text{otherwise,} \end{cases} \tag{3.17b}$$

$$\mathbf{K}(q) := \{(\tilde{\mathbf{u}}_s,\tilde{\mathbf{u}}_\ell) \in \mathbf{V},\ \mathrm{div}_x(\phi_s\tilde{\mathbf{u}}_s + \phi_l\tilde{\mathbf{u}}_\ell) = 0 \text{ a.e. in } \Omega(t)\}. \tag{3.17c}$$

The constraint set $\mathbf{K}(q) \subset \mathbf{V}$ depends on $q = (\chi_s,\chi_\ell) \in \mathbf{Q}$ through ϕ_s,ϕ_ℓ by (3.11). Indeed, with given, fixed ϕ_s,ϕ_ℓ it can be checked that $\mathbf{K}(q)$ is a closed linear subspace of $\mathbf{V}$.

Moreover, in (3.17a) there are the following contributions to the density R

$$R(\phi_s,\phi_\ell;\tilde{\mathbf{u}}_s,\tilde{\mathbf{u}}_\ell,\tilde{e}_s,\tilde{e}_\ell) := R_\ell(\phi_\ell;\tilde{e}_\ell) + R_s(\phi_s;\tilde{e}_s) + R_{s\ell}(\phi_s;\tilde{\mathbf{u}}_s,\tilde{\mathbf{u}}_\ell), \tag{3.17d}$$

$$R_\ell(\phi_\ell;\tilde{e}_\ell) := \tfrac{\tilde{\mu}_{\ell 1}(\phi_\ell)}{2}|\,\mathrm{dev}\,\tilde{e}_\ell|^2 + \tfrac{\tilde{\mu}_{\ell 2}(\phi_\ell)}{2}|\,\mathrm{tr}\tilde{e}_\ell|^2, \tag{3.17e}$$

$$R_{s\ell}(\phi_s;\tilde{\mathbf{u}}_s,\tilde{\mathbf{u}}_\ell) := \tfrac{\tilde{\mu}_{s\ell}(\phi_s)}{2}|\tilde{\mathbf{u}}_s - \tilde{\mathbf{u}}_\ell|^2, \tag{3.17f}$$

$$R_s(\phi_s;\tilde{e}_s) := \tfrac{\tilde{\mu}_s(\phi_s)}{2}\Big[\alpha|\,\mathrm{dev}\,\tilde{e}_s|^2 + \beta_+(\mathrm{tr}\tilde{e}_s)_+^2 + \beta_-(\mathrm{tr}\tilde{e}_s)_-^2 + \gamma|\tilde{e}_s|(\mathrm{tr}\tilde{e}_s)_-\Big], \tag{3.17g}$$

where $e_i = e(\mathbf{u}_i)$, $\tilde{e}_i = e(\tilde{\mathbf{u}}_i)$, $e(\mathbf{u}) := \frac{1}{2}(\nabla\mathbf{u} + \nabla\mathbf{u}^\top)$ is the symmetric strain tensor, $\mathrm{tr}e_i := \sum_{k=1}^d e_{i,kk}$ is the trace of the matrix $e_i = (e_{i,kl})_{k,l=1}^d \in \mathbb{R}^{d\times d}$, and with the notation $\mathrm{dev}\,e_i := e_i - \frac{1}{d}\,\mathrm{tr}e_i\mathbb{I}$ we indicate its deviator. The functions $(\cdot)_\pm$ in (3.17g) denote the positive, resp. negative part, i.e.,

$$(a)_\pm := \max\{\pm a, 0\} \quad \text{for } a \in \mathbb{R}.$$

Observe that the contribution of the liquid (3.17e) and the coupled part (3.17f) are both quadratic, hence convex for strictly positive coefficient functions. Instead, the dissipation potential of the solid phase features, in addition to the quadratic terms, also the mixed term $|\operatorname{dev}\tilde{e}_s|(\operatorname{tr}\tilde{e}_s)_-$. Hence, convexity of the solid dissipation potential can only be ensured under additional assumptions on α, β_-, and γ.

We now specify conditions on the coefficients in (3.17), for which coercivity and convexity of $\mathcal{R}$ can be ensured. Under these conditions we give a characterization of its subdifferential.

Proposition 3.1 (Properties of $\mathcal{R}$) *Let $\mathcal{R}$ be given by (3.17) with the velocity space $\mathbf{V}$ as in (3.15) and let the states $q = (\chi_s, \chi_\ell)$ be given in accordance with (3.6) and (3.11). For given $\mathbf{u}_s \in H^1(\Omega(t);\mathbb{R}^d)$, resp. $\mathbf{u}_\ell \in H^1(\Omega(t);\mathbb{R}^d)$ with $\mathbf{u}_s = \mathbf{u}_\ell = 0$ on $\partial\Omega(t)\backslash\Gamma(t)$, set*

$$\mathbf{V}_{\mathbf{u}_s} := \{\tilde{\mathbf{u}}_\ell \in H^1(\Omega(t);\mathbb{R}^d),\ (\mathbf{u}_s, \tilde{\mathbf{u}}_\ell) \in \mathbf{K}(q)\}\,, \tag{3.18a}$$

$$\mathbf{V}_{\mathbf{u}_\ell} := \{\tilde{\mathbf{u}}_s \in H^1(\Omega(t);\mathbb{R}^d),\ (\tilde{\mathbf{u}}_s, \mathbf{u}_\ell) \in \mathbf{K}(q)\}\,. \tag{3.18b}$$

1. *Assume that $\tilde{\mu}_s, \tilde{\mu}_\ell, \tilde{\mu}_{s\ell} \in L^\infty(\mathbb{R})$ and that there is a constant $\tilde{\mu}_* > 0$ such that $\tilde{\mu}_s, \tilde{\mu}_{\ell 1}, \tilde{\mu}_{\ell 2}, \tilde{\mu}_{s\ell} > \tilde{\mu}_*$ a.e. in $\mathbb{R}$. Further assume that $\alpha, \beta_+, \beta_- > 0$, and $\gamma \geq 0$. Then, for given $q \in \mathbf{Q}$ the functional $\mathcal{R}(q;\cdot)$ is lower semicontinuous and coercive on $\mathbf{V}$, i.e., for all $(\mathbf{u}_s, \mathbf{u}_\ell) \in \mathbf{V}$ it is*

$$\mathcal{R}(q;\dot{q}) \geq \tfrac{1}{2}\tilde{\mu}_*\alpha_* C_{\mathrm{PF}}\big(\|\mathbf{u}_s\|^2_{H^1(\Omega(t);\mathbb{R}^d)} + \|\mathbf{u}_\ell\|^2_{H^1(\Omega(t);\mathbb{R}^d)}\big), \tag{3.19}$$

   where $\alpha_* := \min\{\alpha, \beta_-, \beta_+\}$ and C_{PF} is the Poincaré-Friedrichs constant for $\mathbf{V}$.
2. *Let the assumptions of Item 1. hold true. Then the functional $\mathcal{R}_s(q;\cdot) := \int_{\Omega(t)} R_s(q; e(\cdot))\,\mathrm{d}x$ with R_s from (3.17g) is strictly convex on $\mathbf{V}_{\mathbf{u}_\ell}$, cf. (3.18b), if $\frac{\gamma^2}{(1-\delta)\beta_-} \leq 4\min\{\alpha, \beta_+, \delta\beta_-\}$ for a constant $\delta \in (0,1)$.*
3. *Let the assumptions of Item 1. hold. Then $\mathcal{R}(q;\cdot)$ is strictly convex if $\frac{\gamma^2}{(1-\delta)\beta_-} \leq 4\min\{\alpha, \beta_+, \delta\beta_-\}$ for a constant $\delta \in (0,1)$.*
4. *Let the assumptions of Item 3. hold true. The subdifferential of $\mathcal{R}(q;\cdot)$ for an element $(\mathbf{u}_s, \mathbf{u}_\ell) \in \mathbf{V}$ is given by the elements $(\xi_s, \xi_\ell) + (\zeta_s, \zeta_\ell) \in \mathbf{V}^*$ such that for all $(\tilde{\mathbf{u}}_s, \tilde{\mathbf{u}}_\ell) \in \mathbf{V}$ it is*

$$\mathcal{R}(q;\dot{\tilde{q}}) - \mathcal{R}(q;\dot{q}) \geq \langle(\xi_s + \zeta_s, \xi_\ell + \zeta_\ell), (\tilde{\mathbf{u}}_s, \tilde{\mathbf{u}}_\ell)\rangle_{\mathbf{V}},$$

   with $(\zeta_s, \zeta_\ell) \in \partial\mathcal{I}_{\mathbf{K}(q)}(\mathbf{u}_s, \mathbf{u}_\ell)$ characterized for any $(\mathbf{u}_s, \mathbf{u}_\ell) \in \mathbf{K}(q)$ by elements $\pi \in L^2(\Omega(t))$ in the following way

$$0 = \langle(\zeta_s, \zeta_\ell), (\tilde{\mathbf{u}}_s, \tilde{\mathbf{u}}_\ell)\rangle_{\mathbf{V}} = \int_{\Omega(t)} \pi \operatorname{div}_x(\phi_s\tilde{\mathbf{u}}_s + \phi_l\tilde{\mathbf{u}}_\ell)\,\mathrm{d}x \quad \text{for all } (\tilde{\mathbf{u}}_s, \tilde{\mathbf{u}}_\ell) \in \mathbf{K}(q)\,. \tag{3.20a}$$

Moreover, the elements $(\xi_s, \xi_\ell) \in \mathbf{V}^*$ *are given by*

$$\langle \xi_\ell, \tilde{\mathbf{u}}_\ell \rangle_{H^1(\Omega(t);\mathbb{R}^d)} := \int_{\Omega(t)} \Big[\tilde{\mu}_{\ell 1}(\phi_s)\, \mathrm{dev}\, e_\ell : \mathrm{dev}\, \tilde{e}_\ell + \tilde{\mu}_{\ell 2}(\phi_s)\, \mathrm{tr} e_\ell\, \mathrm{tr} \tilde{e}_\ell - \tilde{\mu}_{s\ell}(\phi_s)(\mathbf{u}_s - \mathbf{u}_\ell) \cdot \tilde{\mathbf{u}}_\ell \Big]\, \mathrm{d}x, \tag{3.20b}$$

$$\begin{aligned} \langle \xi_s, \tilde{\mathbf{u}}_s \rangle_{H^1(\Omega(t);\mathbb{R}^d)} := \int_{\Omega(t)} \Big[& \tilde{\mu}_s(\phi_s)\alpha\, \mathrm{dev}\, e_s : \mathrm{dev}\, \tilde{e}_s + \tilde{\mu}_{s\ell}(\phi_s)(\mathbf{u}_s - \mathbf{u}_\ell) \cdot \tilde{\mathbf{u}}_s \\ & + \hat{\beta}_+ (\, \mathrm{tr} e_s)_+\, \mathrm{tr} \tilde{e}_s + \hat{\beta}_- (\, \mathrm{tr} e_s)_-\, \mathrm{tr} \tilde{e}_s \\ & + \hat{\mu}_1 |e_s|\, \mathrm{tr} \tilde{e}_s + \hat{\mu}_2(e_s) : \tilde{e}_s (\, \mathrm{tr} e_s)_- \Big]\, \mathrm{d}x, \end{aligned} \tag{3.20c}$$

$$\begin{aligned} &\textit{with } \hat{\beta}_+ \in L^\infty(\Omega(t)), && \hat{\beta}_+ = \beta_+ \tilde{\mu}_s(\phi_s) H(\, \mathrm{tr} e_s), \\ &\textit{and } \hat{\beta}_- \in L^\infty(\Omega(t)), && \hat{\beta}_- = -\beta_- \tilde{\mu}_s(\phi_s) H(-\, \mathrm{tr} e_s), \\ &\textit{and } \hat{\mu}_1 \in L^\infty(\Omega(t)), && \hat{\mu}_1 = -\tfrac{\tilde{\mu}_s(\phi_s)\gamma}{2} H(-\, \mathrm{tr} e_s), \\ &\textit{and } \hat{\mu}_2 \in L^\infty(\Omega(t); \mathbb{R}^{d\times d}), && \hat{\mu}_2(e_s) = \begin{cases} \frac{e_s}{|e_s|} \frac{\tilde{\mu}_s(\phi_s)\gamma}{2} \textit{ if } |e_s| > 0, \\ \hat{e} \in \mathbb{R}^{d\times d}_{\mathrm{sym}} \textit{ with } |\hat{e}| \le \frac{\tilde{\mu}_s(\phi_s)\gamma}{2} \textit{ if } |e_s| = 0, \end{cases} \end{aligned}$$

at a.e. point $x \in \Omega(t)$*, and where* H *denotes the Heaviside function*

$$H(a) \in \begin{cases} \{0\} & \textit{if } a < 0, \\ [0,1] & \textit{if } a = 0, \\ \{1\} & \textit{if } a > 0. \end{cases} \tag{3.21}$$

Proof **To 1.:** Observe that the functional $\mathcal{R}(q; \cdot)$ is continuous in $\mathbf{K}(q)$ due to the closedness of this subspace in $\mathbf{V}$. In particular this is immediate for all the quadratic contributions of the functional; the continuity of the product term can be seen by the following calculation

$$\begin{aligned} &\left| \int_{\Omega(t)} \tfrac{\tilde{\mu}_s(\phi_s)}{2} \big(|e_s| (\, \mathrm{tr} e_s)_- - |\tilde{e}_s| (\, \mathrm{tr} \tilde{e}_s)_- \big)\, \mathrm{d}x \right| \\ &\le \tilde{\mu}^* \int_{\Omega(t)} \big| |e_s| - |\tilde{e}_s| \big| \big| (\, \mathrm{tr} e_s)_- - (\, \mathrm{tr} \tilde{e}_s)_- \big|\, \mathrm{d}x \\ &\le \tilde{\mu}^* \| e_s - \tilde{e}_s \|_{L^2(\Omega(t);\mathbb{R}^{d\times d})} \| (\, \mathrm{tr} e_s)_- - (\, \mathrm{tr} \tilde{e}_s)_- \|_{L^2(\Omega(t))} \end{aligned}$$

by Hölder's inequality. This proves continuity in $\mathbf{K}(q)$. Lower semicontinuity in $\mathbf{V}$ then follows by the fact that $\mathcal{R}(q; \mathbf{u}_s, \mathbf{u}_\ell) = \infty$ for any $(\mathbf{u}_s, \mathbf{u}_\ell) \in \mathbf{V} \setminus (\mathbf{V}_{\mathbf{u}_\ell} \times \mathbf{V}_{\mathbf{u}_s})$.

Coercivity estimate (3.19) directly follows from all quadatic terms thanks to the positive bounds from below for the coefficient functions and by Poincaré-Friedrich's inequality in $\mathbf{V}$.

To 2.: Let $(\mathbf{u}_s, \mathbf{u}_\ell), (\tilde{\mathbf{u}}_s, \tilde{\mathbf{u}}_\ell) \in \mathbf{V}$ and $\lambda \in (0,1)$. In what follows, we abbreviate $e = e_s$ and $\tilde{e} = \tilde{e}_s$. First of all, we observe that the positive and the negative part $(\cdot)^\pm$ are convex functions so that $(\lambda\,\mathrm{tr}e + (1-\lambda)\,\mathrm{tr}\tilde{e})^\pm \leq \lambda(\mathrm{tr}e)^\pm + (1-\lambda)(\mathrm{tr}\tilde{e})^\pm$. Since $|\cdot|^2$ is monotone, we find

$$\beta_\pm|(\mathrm{tr}(\lambda e + (1-\lambda)\tilde{e}))^\pm|^2 \leq \beta_\pm|\lambda(\mathrm{tr}e)^\pm + (1-\lambda)(\mathrm{tr}\tilde{e})^\pm|^2 . \tag{3.22}$$

Furthermore, dev and tr are linear operators. Hence, with placeholders $a \in \{\mathrm{dev}\,e, \mathrm{tr}e, (\mathrm{tr}e)_\pm\}$ and $\tilde{a} \in \{\mathrm{dev}\,\tilde{e}, \mathrm{tr}\tilde{e}, (\mathrm{tr}\tilde{e})_\pm\}$ the uniform convexity of $|\cdot|^2$ can be checked:

$$|\lambda a + (1-\lambda)\tilde{a}|^2 = \lambda|a|^2 + (1-\lambda)|\tilde{a}|^2 - \lambda(1-\lambda)(a-\tilde{a})^2. \tag{3.23}$$

This also proves the convexity of R_ℓ. Moreover, the product term contained in R_s can be estimated by monotonicity of $|\cdot|$ and $(\cdot)_-$, and Young's inequality as follows:

$$\begin{aligned}
&|\lambda e + (1-\lambda)\tilde{e}|(\mathrm{tr}(\lambda e + (1-\lambda)\tilde{e}))_- \\
&\leq (\lambda|e| + (1-\lambda)|\tilde{e}|)(\lambda(\mathrm{tr}e)_- + (1-\lambda)(\mathrm{tr}\tilde{e})_-) \\
&= \lambda|e|(\mathrm{tr}e)_- + (1-\lambda)|\tilde{e}|(\mathrm{tr}\tilde{e})_- \\
&\quad -\lambda(1-\lambda)\big(|e| - |\tilde{e}|\big)\big((\mathrm{tr}e)_- - (\mathrm{tr}\tilde{e})_-\big) \\
&\leq \lambda|e|(\mathrm{tr}e)_- + (1-\lambda)|\tilde{e}|(\mathrm{tr}\tilde{e})_- \\
&\quad +\lambda(1-\lambda)\sqrt{\varepsilon}\big||e| - |\tilde{e}|\big|\big|(\mathrm{tr}e)_- - (\mathrm{tr}\tilde{e})_-\big|(\sqrt{\varepsilon})^{-1} \\
&\leq \lambda|e|(\mathrm{tr}e)_- + (1-\lambda)|\tilde{e}|(\mathrm{tr}\tilde{e})_- \\
&\quad +\lambda(1-\lambda)\big(\tfrac{\varepsilon}{2}\big(|e| - |\tilde{e}|\big)^2 + \tfrac{1}{2\varepsilon}\big((\mathrm{tr}e)_- - (\mathrm{tr}\tilde{e})_-\big)^2\big),
\end{aligned}$$

where the positive terms in the very last line of this estimate have to be absorbed by the corresponding negative term obtained in (3.23). For this, it can be checked that

$$\begin{aligned}
&-\alpha(|\mathrm{dev}\,e| - |\mathrm{dev}\,\tilde{e}|)^2 - \beta_+((\mathrm{tr}e)_+ - (\mathrm{tr}\tilde{e})_+)^2 - (\delta + 1 - \delta)\beta_-((\mathrm{tr}e)_- - (\mathrm{tr}\tilde{e})_-)^2 \\
&\leq -m_\delta(|e| - |\tilde{e}|)^2 - (1-\delta)\beta_-((\mathrm{tr}e)_- - (\mathrm{tr}\tilde{e})_-)^2
\end{aligned}$$

with $m_\delta := \min\{\alpha, \beta_+, \delta\beta_-\}$ for a constant $\delta \in (0,1)$. Thus, combining this estimate with the previous ones, we obtain

$$\begin{aligned}
R_s(\phi_s; \lambda e + (1-\lambda)\tilde{e}) &\leq \lambda R_s(\phi_s; \lambda e) + (1-\lambda)R_s(\phi_s; \tilde{e}) \\
&\quad -\lambda(1-\lambda)\tfrac{\tilde{\mu}(\phi_s)}{2}\big((m_\delta - \tfrac{\gamma\varepsilon}{2})\big(|\mathrm{dev}\,e| - |\mathrm{dev}\,\tilde{e}|\big)^2 \\
&\qquad +((1-\delta)\beta_- - \tfrac{\gamma}{2\varepsilon})\big((\mathrm{tr}e)_- - (\mathrm{tr}\tilde{e})_-\big)^2 + \beta_+\big((\mathrm{tr}e)_+ - (\mathrm{tr}\tilde{e})_+\big)^2\big),
\end{aligned}$$

and we have to make sure that both $m_\delta - \frac{\gamma\varepsilon}{2} \geq 0$ and $(1-\delta)\beta_- - \frac{\gamma}{2\varepsilon} \geq 0$. This implies the constraint $\frac{\gamma}{2(1-\delta)\beta_-} \leq \varepsilon \leq \frac{2m_\delta}{\gamma}$, which finally gives $\frac{\gamma^2}{(1-\delta)\beta_-} \leq 4m_\delta$ for strict convexity.

To 3.: Thanks to the previously proved statement of Item 2, the convexity properties of the full functional $\mathcal{R}(q;\cdot)$ now follow by the uniform convexity of the quadratic fluid and solid-fluid contributions.

To 4.: From Item 1. we recall that $\mathcal{R}(q;\cdot)$ is convex. The Moreau-Rockafellar Theorem for convex functionals, cf. e.g. [17, p. 200, Thm. 1], provides a sum rule for the subdifferential of convex functionals, i.e.: *If* $F_1,\ldots,F_k : U \to (-\infty,\infty]$ *are proper, convex functionals, all but possibly one of them continuous in a point* $\bar{v} \in \mathrm{dom}F_1 \cap \ldots \cap \mathrm{dom}F_k$, *then*

$$\partial F_1(v) + \ldots + \partial F_k(v) = \partial(F_1(v) + \ldots + F_k(v)) \quad \textit{for all } v \in U. \tag{3.24}$$

We observe that all the contributions to $\int_{\Omega(t)} R\,\mathrm{d}x$ are continuous on all of $\mathbf{V}$ and a possible discontinuity for some $(\mathbf{u}_s,\mathbf{u}_\ell) \in \mathrm{dom}\mathcal{R}$ arises by the constraint term $\mathcal{I}_{\mathbf{K}(q)}$. Hence, the prerequisites of the Moreau-Rockafellar Theorem are met and (3.24) applies to determine the contributions of its subdifferential.

In order to find the characterization (3.20a) of $(\zeta_s,\zeta_\ell) \in \partial\mathcal{I}_{\mathbf{K}(q)}(\mathbf{u}_s,\mathbf{u}_\ell)$ we note that for any $(\tilde{\mathbf{u}}_s,\tilde{\mathbf{u}}_\ell) \in \mathbf{V}$ it is

$$(\tilde{\mathbf{u}}_s,\tilde{\mathbf{u}}_\ell) \in \mathbf{K}(q) \quad \Leftrightarrow \quad \text{for all } \eta \in L^2(\Omega(t)) : \int_{\Omega(t)} \eta\,\mathrm{div}_x(\phi_s\tilde{\mathbf{u}}_s + \phi_\ell\tilde{\mathbf{u}}_\ell)\,\mathrm{d}x = 0\,. \tag{3.25}$$

This equivalently states that the annihilator $\mathbf{K}(q)^\perp$ of the linear subspace $\mathbf{K}(q)$ is given by

$$\mathbf{K}(q)^\perp = \Big\{\Big(\int_{\Omega(t)} \eta\,\mathrm{div}_x(\phi_s \bullet + \phi_\ell \bullet)\,\mathrm{d}x\Big) : \mathbf{K}(q) \to 0,\ \eta \in L^2(\Omega(t))\Big\}\,.$$

On the other hand, by the definition of the subdifferential of $\mathcal{I}_{\mathbf{K}(q)}$ for any $(\mathbf{u}_s,\mathbf{u}_\ell) \in \mathbf{K}(q)$ we have that $(\zeta_s,\zeta_\ell) \in \partial\mathcal{I}_{\mathbf{K}(q)}(\mathbf{u}_s,\mathbf{u}_\ell)$ is a support function, i.e.,

$$(\zeta_s,\zeta_\ell) \in \partial\mathcal{I}_{\mathbf{K}(q)}(\mathbf{u}_s,\mathbf{u}_\ell) \quad \Leftrightarrow \quad \text{for all } (\tilde{\mathbf{u}}_s,\tilde{\mathbf{u}}_\ell) \in \mathbf{K}(q) : \langle(\zeta_s,\zeta_\ell),(\mathbf{u}_s,\mathbf{u}_\ell) - (\tilde{\mathbf{u}}_s,\tilde{\mathbf{u}}_\ell)\rangle_{\mathbf{V}} \geq 0\,.$$

With the specific choices $(\tilde{\mathbf{u}}_s,\tilde{\mathbf{u}}_\ell) = (0,0) \in \mathbf{K}(q)$ and $(\tilde{\mathbf{u}}_s,\tilde{\mathbf{u}}_\ell) = -2(\mathbf{u}_s,\mathbf{u}_\ell) \in \mathbf{K}(q)$ we find that $\langle(\zeta_s,\zeta_\ell),(\mathbf{u}_s,\mathbf{u}_\ell)\rangle_{\mathbf{V}} = -\langle(\zeta_s,\zeta_\ell),(\mathbf{u}_s,\mathbf{u}_\ell)\rangle_{\mathbf{V}} \geq 0$ and hence $(\zeta_s,\zeta_\ell) = 0$ on $\mathbf{K}(q)$. This means that $(\zeta_s,\zeta_\ell) \in \mathbf{K}(q)^\perp$ and hence (3.20a) is deduced.

It remains to determine the other contributions to the subdifferential given by (3.20b) & (3.20c). For this, we further make use of the chain rule for the subdifferential of convex functionals, cf. e.g. [17, p. 201, Thm. 2]: *Assume that* $A : U \to W$ *is linear,* $\mathcal{F} : W \to (-\infty,\infty]$ *is convex and there is* $u \in U$ *such that* $\mathcal{F}$ *is continuous in* Au. *Then,*

$$\partial(\mathcal{F} \circ A)(u) = (A^*\partial\mathcal{F})(Au), \tag{3.26}$$

where $A^* : W^* \to U^*$ *is the adjoint of* A, *defined by* $\langle A^*u^*, v\rangle = \langle u^*, Av\rangle$.

Since the dissipation potential of the liquid (3.17e) and the coupling term (3.17f) are Fréchet-differentiable, we directly find (3.20b) and the second summand of

(3.20c). To deduce the remaining terms of (3.20c) we shall apply the above theorem to the dissipation potential of the solid $\mathcal{R}_s(q;\cdot)$. To this aim we set $U = \mathbf{V}_{\mathbf{u}_\ell}$ with given $\mathbf{u}_\ell$, $A : \mathbf{V}_{\mathbf{u}_\ell} \to W = L^2(\Omega(t);\mathbb{R}^{d\times d}) \times L^2(\Omega(t)) \times L^2(\Omega(t);\mathbb{R}^{d\times d})$, $Av := (\operatorname{dev} e(v), \operatorname{tr} e(v), e(v))^\top$ and set $\widetilde{\mathcal{R}}_s(a_1,a_2,a_3) := \int_{\Omega(t)} \frac{\tilde\mu(\phi_s)}{2}\big(\alpha|a_1|^2 + \beta_+|(a_2)_+|^2 + \beta_-|(a_2)_-|^2 + \gamma|a_3|(a_2)_-\big)\,\mathrm{d}x$. Thus, $\mathcal{R}_s(q;v) = (\widetilde{\mathcal{R}}_s \circ A)(v)$ for all $v \in \mathbf{V}_{\mathbf{u}_\ell}$. Thanks to the previously proved continuity and convexity properties of $\mathcal{R}(q;\cdot)$ we see that also $\widetilde{\mathcal{R}}_s$ is convex and continuous on W. Hence chain rule (3.26) is applicable. To ultimately conclude (3.20c), we note that for all $(a_1,a_2,a_3),(\tilde a_1,\tilde a_2,\tilde a_3) \in W$ it is

$$
\begin{aligned}
&\langle \partial\widetilde{\mathcal{R}}_s(a_1,a_2,a_3),(\tilde a_1,\tilde a_2,a_3)\rangle_W \\
&\quad = \langle \partial_{a_1}\widetilde{\mathcal{R}}_s(a_1,a_2,a_3),\tilde a_1\rangle_{L^2(\Omega(t))} + \langle \partial_{a_2}\widetilde{\mathcal{R}}_s(a_1,a_2,a_3),\tilde a_2\rangle_{L^2(\Omega(t))} \quad \text{with} \\
&\langle \partial_{a_1}\widetilde{\mathcal{R}}_s(a_1,a_2,a_3),\tilde a_1\rangle_{L^2(\Omega(t))} = \int_{\Omega(t)} \tilde\mu_s(\phi_s)\alpha a_1 : \tilde a_1\,\mathrm{d}x\,, \\
&\langle \partial_{a_2}\widetilde{\mathcal{R}}_s(a_1,a_2,a_3),\tilde a_2\rangle_{L^2(\Omega(t))} = \int_{\Omega(t)} \big(\hat\beta_+(a_2)_+\tilde a_2 + \hat\beta_-(a_2)_-\tilde a_2 + \hat\mu_1|a_3|\tilde a_2\big)\,\mathrm{d}x\,, \\
&\langle \partial_{a_3}\widetilde{\mathcal{R}}_s(a_1,a_2,a_3),\tilde a_3\rangle_{L^2(\Omega(t))} = \int_{\Omega(t)} (a_2)_-\hat\mu_2(a_3) : \tilde a_3\,\mathrm{d}x\,,
\end{aligned}
$$

with the coefficient functions $\hat\beta_\pm, \hat\mu_1, \hat\mu_2$ as stated in (3.20c). □

In order to state (3.1b) for the system of concentrated suspensions it remains to calculate the derivative of the energy functional.

Proposition 3.2 (Functional derivative of $\mathcal{E}$) *Let the energy functional $\mathcal{E}(q)$ be given as in (3.16) and consider the family of flow maps $q(h)$ defined by*

$$\chi_i(h,X) = X + h\,\mathbf{u}_i(X), \tag{3.27}$$

for any arbitrary $\mathbf{u}_i \in H^1(\bar\Omega;\mathbb{R}^d)$ representing an element $\dot q = (\mathbf{u}_s,\mathbf{u}_\ell) \in \mathbf{V}$. Then the variation of $\mathcal{E}$ in an arbitrary direction $\dot q \in \mathbf{V}$ is given by

$$\langle \mathrm{D}_q\mathcal{E}(q),\dot q\rangle = \lim_{h\to 0}\frac{1}{h}\big[\mathcal{E}\big(q(h)\big) - \mathcal{E}\big(q(0)\big)\big]\,. \tag{3.28}$$

1. *The functional derivative of $\mathcal{E}_{\text{bulk}}$ from (3.16a) reads*

$$\langle \mathrm{D}_q\mathcal{E}_{\text{bulk}}(q),\dot q\rangle = \int_\Omega (\nabla_x E)\cdot\mathbf{u}_s + (E - \phi_s\partial_{\phi_s}E)(\nabla\cdot\mathbf{u}_s)\,\mathrm{d}x \tag{3.29}$$

where $E = E(x,\phi_s)$.

2. *The functional derivative of $\mathcal{E}_{\text{surf}}$ from (3.16c) reads*

$$\langle \mathrm{D}_q\mathcal{E}_{\text{surf}}(q),\dot q\rangle = \int_\Gamma \Big(\mathbf{u}\cdot\nabla_x\vartheta + \vartheta\,\mathrm{div}_\Gamma(\mathbf{u})\Big)\,\mathrm{d}\mathcal{H}^{d-1} \tag{3.30}$$

with surface energy $\vartheta = \vartheta(x)$ and $\mathbf{u} = \phi_s\mathbf{u}_s + \phi_\ell\mathbf{u}_\ell$.

Proof **To 1.:** First we use change of variables to express the integral

$$\mathcal{E}_{\text{bulk}}\big(q(h)\big) = \int_{\Omega(h)} E\big(x, \phi_s(h,x)\big)\,\mathrm{d}x$$
$$= \int_{\bar{\Omega}} E\left(\chi_s(h,X), \frac{\bar{\phi}_s(X)}{\det F_s(h,X)}\right) \det F_s(h,X)\,\mathrm{d}X.$$

This allow us to use (3.28) for a fixed domain. Then the differentiation of the integrand gives the expression

$$\langle \mathrm{D}_q \mathcal{E}_{\text{bulk}}(q), \dot{q}\rangle = \int_{\bar{\Omega}} \lim_{h\to 0} \frac{1}{h}\left[E\left(\chi_s(h,X), \tfrac{\bar{\phi}_s(X)}{\det F_s(h,X)}\right)\det F_s(h,X) - E\left(X, \bar{\phi}_s(X)\right)\right]\mathrm{d}X$$
$$= \int_{\bar{\Omega}} (\nabla_x E)\cdot \mathbf{u}_s + \left[(\partial_{\phi_s} E)\left(-\frac{\bar{\phi}_s}{\det F_s}\right) + E\right](\partial_h \det F_s)_{h=0}\,\mathrm{d}X$$
$$= \int_{\bar{\Omega}} (\nabla_x E)\cdot \mathbf{u}_s + (E - \phi_s \partial_{\phi_s} E)\nabla\cdot \mathbf{u}_s\,\mathrm{d}x$$

where at $h = 0$ we have $x \equiv X$. We used a simple version of Jacobi's formula $\partial_h \det F_s = (\det F_s)\,\mathrm{tr}(F_s^{-1}\partial_h F_s)$, $\det F_s = 1$, and $\mathrm{tr}\partial_h F_s = \nabla\cdot \mathbf{u}_s$ for $h = 0$. The result remains valid for arbitrary q if the final integral is expressed in x-coordinates.

To 2.: We use again change of variables to express the integrals

$$\mathcal{E}_{\text{surf}}(q(h)) = \int_{\Gamma(h)} \vartheta(x)\,\mathrm{d}\mathcal{H}^{d-1} = \int_{\bar{\Gamma}} \vartheta(\chi_i(t,X))\|\mathrm{Cof}(F_i(t,X))\cdot \mathbf{n}\|\,\mathrm{d}\mathcal{H}^{d-1},$$

where $\mathrm{Cof} F_i = (\det F_i)(F_i^{-1})^\top$ is the cofactor of the Jacobian. The differentiation of this term is slightly more technical and can be found, for instance, in [30]. The resulting expression is

$$\langle \mathcal{E}_{\text{surf}}, \dot{q}\rangle = \int_{\Gamma} (\mathbf{u}\cdot\nabla_x\vartheta + \vartheta\,\mathrm{div}_\Gamma\,\mathbf{u})\,\mathrm{d}\mathcal{H}^{d-1},$$

where we used the surface divergence $\mathrm{div}_\Gamma\,\mathbf{u}$. Observe that via the *divergence theorem on manifolds* one can rewrite

$$\int_\Gamma \mathrm{div}_\Gamma\,\mathbf{u}\,\mathrm{d}s = -\int_\Gamma \mathbf{H}\cdot\mathbf{u}\,\mathrm{d}s, \tag{3.31}$$

where $\mathbf{H} = H\mathbf{n} \equiv -\mathbf{n}(\nabla_\Gamma\cdot\mathbf{n})$ is the mean curvature vector and H the scalar mean curvature (with respect to $\mathbf{n}$). Also note that $\mathbf{u}$ can be replaced with $\mathbf{u}_s$ or $\mathbf{u}_\ell$ since by (3.6d) they all agree on Γ for a given variation $\dot{q}$. □

3.3 PDE system obtained by the gradient flow formulation

In this section we combine the results of Propositions 3.1 & 3.2 in order to obtain formulation of the force balance (3.1b) for the problem.

Weak formulation of the problem.

Force balance (3.1b)

$$-\mathrm{D}\mathcal{E}(q) \in \partial\mathcal{R}(\dot{q}) \quad \text{in } \mathbf{V}^*$$

is now directly obtained from the results of Propositions 3.1 & 3.2. For shorter notation we observe that the gradient terms arising in the differential of the bulk dissipation, cf. (3.20), define viscous stresses of solid and liquid phase. We here gather them in terms of the stress tensors σ_s, σ_ℓ given by

$$\sigma_\ell = \tilde{\mu}_{\ell 1}\ \mathrm{dev}(e(\mathbf{u}_\ell)) + \tilde{\mu}_{\ell 2}\ \mathrm{tr}(e(\mathbf{u}_\ell))\mathbb{I}, \tag{3.32a}$$

$$\sigma_s = \tilde{\mu}_s \alpha\ \mathrm{dev}(e(\mathbf{u}_s)) + \big[\hat{\beta}_+(\,\mathrm{tr}e(\mathbf{u}_s))_+ + \hat{\beta}_-(\,\mathrm{tr}e(\mathbf{u}_s))_- + \hat{\mu}_1|e(\mathbf{u}_s)|\big]\mathbb{I} + \sigma_s^*, \tag{3.32b}$$

$$\sigma_s^* = \hat{\mu}_2(e(\mathbf{u}_s))(\,\mathrm{tr}e(\mathbf{u}_s))_-, \tag{3.32c}$$

where the coefficient functions $\hat{\beta}_\pm, \hat{\mu}_1, \hat{\mu}_2$ are defined in (3.20c). In this way, the weak formulation induced by (3.1b) reads as follows:

$$\begin{aligned}
&\langle(\xi_s + \zeta_s, \xi_\ell + \zeta_\ell), (\tilde{\mathbf{u}}_s, \tilde{\mathbf{u}}_\ell)\rangle_{\mathbf{V}} \\
&= \int_{\Omega(t)} \sigma_\ell : e(\tilde{\mathbf{u}}_\ell) + \sigma_s : e(\tilde{\mathbf{u}}_s) + \tilde{\mu}_{s\ell}(\mathbf{u}_\ell - \mathbf{u}_s)\cdot(\tilde{\mathbf{u}}_\ell - \tilde{\mathbf{u}}_s) + \pi\,\mathrm{div}_x(\phi_s\tilde{\mathbf{u}}_s + \phi_\ell\tilde{\mathbf{u}}_\ell)\,\mathrm{d}x \\
&= -\int_{\Omega(t)} (\nabla_x E)\cdot\tilde{\mathbf{u}}_s - \pi_s\,\mathrm{div}_x\,\tilde{\mathbf{u}}_s\,\mathrm{d}x - \int_{\Gamma(t)} \vartheta\,\mathrm{div}_\Gamma\,\tilde{\mathbf{u}}\,\mathrm{d}\mathcal{H}^{d-1} = -\langle \mathrm{D}\mathcal{E}(q), (\tilde{\mathbf{u}}_s, \tilde{\mathbf{u}}_\ell)\rangle_{\mathbf{V}}\,,
\end{aligned} \tag{3.33}$$

for all $(\tilde{\mathbf{u}}_s, \tilde{\mathbf{u}}_\ell) \in \mathbf{V}$, with $\pi_s := -(E - \phi_s\partial_{\phi_s}E)$ as an effective pressure of the solid phase, $\tilde{\mathbf{u}} = \phi_s\tilde{\mathbf{u}}_s + \phi_\ell\tilde{\mathbf{u}}_\ell$, and with $(\xi_s + \zeta_s, \xi_\ell + \zeta_\ell) \in \partial\mathcal{R}(q, \dot{q})$.

Pointwise formulation of the problem.

Suppose now that all the functions involved in (3.33) are sufficiently smooth, so that we can integrate by parts in (3.33) in order to move the gradients from the test functions to the stress and pressure terms. This leads to the classical, pointwise formulation of the problem, again involving the stresses σ_ℓ, σ_s from (3.32).

In order to reconstruct the pointwise PDE formulation we first rewrite the derivative of $\mathcal{E}_{\text{bulk}}$ as

$$\begin{aligned}\langle \mathrm{D}_q \mathcal{E}_{\text{bulk}}(q), \dot{q}\rangle &= \int_\Omega (\nabla_x E)\cdot \tilde{\mathbf{u}}_s + (E - \phi_s \partial_{\phi_s} E)(\nabla \cdot \tilde{\mathbf{u}}_s)\,\mathrm{d}x \\ &= \int_\Omega (\nabla_x E + \nabla p^*)\cdot \tilde{\mathbf{u}}_s \,\mathrm{d}x + \int_{\partial\Omega} (-p^*)\tilde{\mathbf{u}}_s \cdot \mathbf{n}\,\mathrm{d}\mathcal{H}^{d-1}, \end{aligned} \tag{3.34a}$$

where the effective pressure is defined

$$p^*(x,\phi_s) = \phi_s \partial_{\phi_s} E(x,\phi_s) - E(x,\phi_s). \tag{3.34b}$$

The derivative of $\mathcal{E}_{\text{surf}}$ we already characterized in (3.31) using the mean curvature.

In particular, for all $t \in [0,T]$, a.e. in $\Omega(t)$ the following PDE-system has to be satisfied:

$$-\operatorname{div}_x \sigma_s + \tilde{\mu}_{s\ell}(\mathbf{u}_s - \mathbf{u}_\ell) = -\phi_s \nabla(\pi + \pi_s), \tag{3.35a}$$
$$-\operatorname{div}_x \sigma_\ell - \tilde{\mu}_{s\ell}(\mathbf{u}_s - \mathbf{u}_\ell) = -\phi_\ell \nabla\pi, \tag{3.35b}$$
$$\operatorname{div}_x \left(\phi_s \mathbf{u}_s + \phi_\ell \mathbf{u}_\ell\right) = 0, \tag{3.35c}$$

together with the following boundary conditions:

$$(\sigma_s + \sigma_\ell)\,\mathbf{n} = (d-1)\vartheta\kappa + \pi + \pi_s \quad \text{on } \Gamma(t)\,, \tag{3.35d}$$
$$\mathbf{u}_\ell = \mathbf{u}_s \quad \text{on } \Gamma(t)\,, \tag{3.35e}$$
$$\mathbf{u}_\ell = \mathbf{u}_s = 0 \quad \text{on } \partial\Omega(t)\backslash\Gamma(t)\,. \tag{3.35f}$$

Comparison of models.

Even though the model in (3.35) already appears very similar to the one in (2.1), we perform a short discussion on the terms in the stress and the pressures. Firstly, the gradient flow model (3.35) offers a systematic way to include forces due to bulk energies $\mathcal{E}_{\text{bulk}}$ and surface energies and $\mathcal{E}_{\text{surf}}$, leading to the coupling term p^*, p_s and the corresponding boundary terms in (3.35d). The easiest to identify are the pressure terms in (3.35), if we decompose the contribution $\sigma_s - \sigma_s^*$ to the solid stress into a volumetric and a deviatoric part

$$\sigma_s - \sigma_s^* := -p_s \mathbb{I} + 2\mu_s^* \operatorname{dev} \mathbb{D}\mathbf{u}_s \tag{3.36a}$$

with

$$\mu_s^* = \frac{1}{2}\tilde{\mu}_s \alpha, \tag{3.36b}$$

$$p_s = -\beta_+(\operatorname{div}_x \mathbf{u}_s)_+ - \beta_-(\operatorname{div}_x \mathbf{u}_s)_- - \hat{\mu}_1|\mathbb{D}\mathbf{u}_s| \overset{\operatorname{div}_x \mathbf{u}_s = 0}{=} \frac{\gamma}{2}\tilde{\mu}_s(\phi_s)|\mathbb{D}\mathbf{u}_s| H(-\operatorname{div}_x \mathbf{u}_s), \tag{3.36c}$$

where we used the material law $\hat{\mu}_1 = -\frac{\gamma}{2}\tilde{\mu}_s H(-\operatorname{div}_x \mathbf{u}_s)$ with the Heaviside function H as defined in (3.21). Note that H is mutli-valued in $\operatorname{div}_x \mathbf{u}_s = 0$ with $H(0) \in [0,1]$.

In order to compare this with stresses p_c, τ_s in (2.1) we have to identify

$$-p_c\mathbb{I} + \phi_s\tau_s \stackrel{!}{=} -p_s\mathbb{I} + 2\mu_s^* \operatorname{dev}\mathbb{D}(\mathbf{u}_s). \tag{3.37}$$

with p_s, μ_s^* from (3.36). This shows how the normal pressure p_c emerges from p_s in (3.36c) and also gives rise to a novel coupling term σ_s^* from (3.32c), i.e.,

$$\sigma_s^* = \begin{cases} \frac{e_s}{|e_s|}\frac{\tilde{\mu}_s(\phi_s)\gamma}{4}(\operatorname{tr} e_s)_- & \text{if } |e_s| > 0, \\ 0 \in \mathbb{R}^{d\times d}_{\mathrm{sym}} & \text{if } |e_s| = 0. \end{cases} \tag{3.38}$$

The comparison for liquid stresses is entirely similar.

4 Conclusion

This paper focusses on a two-phase model that was derived in [1] using the general averaging approach introduced in [10, 11]. The key ingredient is a stress-strain relation that features a normal pressure p_c which is proportional to the solid shear rate $|\mathbb{D}(\mathbf{u}_s)|$ and becomes singular as the solid volume fraction approaches a critical value $\phi_s \to \phi_{\mathrm{crit}}$. In stationary shear flow situations with prescribed normal pressure p_c this produces a yield threshold due to zones where $\phi_s = \phi_{\mathrm{crit}}$. This law extends a rheological relation inferred by [5] from scaling arguments and experimental measurements of constant shear flow to the general case where the average liquid and solid phase flow fields can be different. Unfortunately, previous investigations also showed that even in these simple flow situations the equations are not well-posed suggesting that some physics is missing.

In this paper, we reformulate the model within a variational framework based on the concepts of gradient flows and energy dissipation. This allows us to infer useful properties about the model and, as a long-term goal, access the rich analytical machinery that has been developed for models formulated within this framework. For example, we can deduce a general form of the normal pressure which includes the relation formulated in [1]. In fact, we observe that the model creates a novel contribution σ_s^* to the solid shear stress σ_s. The dissipation potential is only ensured to be convex for certain parameter ranges $(\alpha, \beta_\pm, \gamma)$, thus offering an analytical reason for the loss of well-posedness that may provide clues which kind of additional physics is required. Thus, we provide an alternative route for discussing this phenomenon which has also been observed for granular flow models based on the similar $\mu(I)$ rheology [2, 3]. Moreover, the variational framework provides appropriate boundary conditions for free interfaces of the suspension.

References

1. Ahnert, T., Münch, A., Wagner, B.: Models for the two-phase flow of concentrated suspensions. European Journal of Applied Mathematics pp. 1–33 (2018).
2. Barker, T., Schaeffer, D.G., Bohorquez, P., Gray, J.M.N.T.: Well-posed and ill-posed behaviour of the μ(I)-rheology for granular flow. Journal of Fluid Mechanics **779**, 794–818 (2015).
3. Barker, T., Schaeffer, D.G., Shearer, M., Gray, J.M.N.T.: Well-posed continuum equations for granular flow with compressibility and μ(I)-rheology. Proc. R. Soc. A **473**, 20160846 (2017).
4. Batchelor, G.K., Green, J.T.: The determination of the bulk stress in a suspension of spherical particles to order c^2. J. Fluid Mech. **56**(03), 401–427 (1972).
5. Boyer, F., Guazzelli, É., Pouliquen, O.: Unifying suspension and granular rheology. Phys. Rev. Lett. **107**(18), 188301 (2011).
6. Brennen, C.: Fundamentals of Multiphase Flow. Cambridge University Press (2005)
7. Cassar, C., Nicolas, M., Pouliquen, O.: Submarine granular flows down inclined planes. Phys. Fluids **17**(10), 103301 (2005).
8. DeGiuli, E., Düring, G., Lerner, E., Wyart, M.: Unified theory of inertial granular flows and non-Brownian suspensions. Physical Review E **91**(6) (2015).
9. Drew, D.: Mathematical modeling of two-phase flow. Annu. Rev. Fluid Mech. **15**(1), 261–291 (1983).
10. Drew, D., Passman, S.: Theory of Multicomponent Fluids, *Applied Mathematical Sciences*, vol. 135. Springer (1999).
11. Drew, D., Segel, L.: Averaged equations for two-phase media. Stud. Appl. Math. **50**(2), 205–231 (1971)
12. Einstein, A.: Eine neue Bestimmung der Moleküldimensionen. Ann. Phys. (Berlin) **324**(2), 289–306 (1905).
13. Giga, M.H., Kirshtein, A., Liu, C.: Variational modeling and complex fluids. Handbook of Mathematical Analysis in Mechanics of Viscous Fluids pp. 73–113 (2018)
14. Grmela, M., Öttinger, H.: Dynamics and thermodynamics of complex fluids. i. development of a general formalism. Physical Review E **56**(6), 6620 (1997)
15. Helmholtz, H.v.: Zur Theorie der stationären Ströme in reibenden Flüssigkeiten. Wiss. Abh. **1**, 223–230 (1868)
16. Hermes, M., Guy, B., Poon, W., Poy, G., Cates, M., Wyart, M.: Unsteady flow and particle migration in dense, non-Brownian suspensions. Journal of Rheology **60**(5), 905–916 (2016).
17. Ioffe, A.D., Tihomirov, V.M.: Theory of extremal problems, *Studies in Mathematics and its Applications*, vol. 6. North-Holland Publishing Co., Amsterdam (1979). Translated from the Russian by Karol Makowski
18. Ishii, M., Hibiki, T.: Thermo-Fluid Dynamics of Two-Phase Flow. Springer (2011).
19. James, N., Han, E., Jureller, J., Jaeger, H.: Interparticle hydrogen bonding can elicit shear jamming in dense suspensions. arXiv:1707.09401 [cond-mat] (2017).
20. Joseph, D., Renardy, Y.: Fundamentals of two-fluid dynamics: Part i: Mathematical theory and applications, vol. 3. Springer Science & Business Media (2013)
21. Krieger, I., Dougherty, T.: A mechanism for non-newtonian flow in suspensions of rigid spheres. Transactions of the Society of Rheology **3**(1), 137–152 (1959).
22. Mielke, A.: On evolutionary Gamma convergence for gradient systems. In: A.Z. A. Muntean J.D.M. Rademacher (ed.) Macroscopic and Large Scale Phenomena: Coarse Graining, Mean Field Limits and Ergodicity, *Lecture Notes in Applied Mathematics and Mechanics*, vol. 3, pp. 187–249. Springer International Publishing, Heidelberg et al. (2016)
23. Mielke, A., Roubíček, T.: Rate-independent Systems: Theory and Application, *Applied Mathematical Sciences*, vol. 193. Springer (2015)
24. Morris, J., Boulay, F.: Curvilinear flows of noncolloidal suspensions: The role of normal stresses. J. Rheol. **43**, 1213–1237 (1999).
25. Morrison, P.J.: Hamiltonian description of the ideal fluid. Reviews of Modern Physics **70**, 467–521 (1998).

26. Murisic, N., Pausader, B., Peschka, D., Bertozzi, A.L.: Dynamics of particle settling and resuspension in viscous liquid films. J. Fluid Mech. **717**, 203–231 (2013).
27. Oh, S., Song, Y., Garagash, D., Lecampion, B., Desroches, J.: Pressure-Driven Suspension Flow near Jamming. Physical Review Letters **114**(8) (2015).
28. Öttinger, H., Grmela, M.: Dynamics and thermodynamics of complex fluids. ii. illustrations of a general formalism. Physical Review E **56**(6), 6633 (1997)
29. Peletier, M.: Variational modelling: Energies, gradient flows, and large deviations. arXiv:1402.1990 (2014)
30. Sokolowski, J., Zolesio, J.P.: Introduction to shape optimization. In: Introduction to Shape Optimization, pp. 5–12. Springer (1992)
31. Strutt, J.: Some general theorems relating to vibrations. Proceedings of the London Mathematical Society **1**(1), 357–368 (1871)
32. Wyart, M., Cates, M.E.: Discontinuous shear thickening without inertia in dense non-brownian suspensions. Phys. Rev. Lett. **112**, 098302 (2014).