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Modeling the shape dynamics of suspensions of permeable ellipsoidal particles

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ABSTRACT

A dynamic two-scale model is developed for describing the mechanical behavior of suspensions of permeable ellipsoidal particles. The particle dynamics in the proposed model is described in terms of particle positions as well as conformation tensors that capture their size, shape, and orientation. Using non-equilibrium thermodynamics, the macroscopic fluid-dynamics and the particle dynamics on the microstructural level are mutually coupled in a consistent manner. So doing, the link between the macroscopic behavior, e.g. stresses, and the dynamics of the microstructure, e.g. particle shape and size, is established. Finally, the model is cast into a form in which the shape tensor is split into its volumetric and isochoric shape contributions, making it possible to model particles with both shape-preserving size-changes (e.g. swellable particles) and volume-preserving shape-changes (e.g. incompressible yet deformable particles). The size-shape model distinguishes itself in unifying prior knowledge of purely-shape models with that of purely-size models by appropriate choices of the Helmholtz free energy and the generalized mobility.

1. Introduction

A wide variety of applications nowadays relies on materials where their overall properties can be tailored to meet specific requirements. Soft, permeable particle suspensions provide the versatility required to achieve exactly this purpose, making them particularly useful in paints and inks [1,2], pharmaceuticals and cosmetics [3,4], and foods [5]. The fascinating properties of the overall suspension emanate primarily from the properties of the individual particles. On the one hand, the elasticity of the supporting network of the individual particle gives rise to its elastic behavior. The flow of the viscous suspending solvent through this elastic network, on the other hand, results in its viscoelastic behavior.

The rich behavior of permeable-particle suspensions emerges from the fact that permeable particles can undergo size and shape changes in response to different stimuli. For instance, permeable particles in a sufficiently-jammed state undergo rate-dependent volume changes as the viscous background solvent is expelled from the interior of the particle [6,7]. The shape changes in permeable particles are induced by steric effects in concentrated suspensions as a particle impinges against neighboring particles [7]. While elastic shape-changes can be accounted for through soft-interaction potentials [8–10], the effect of the viscous background solvent on both the shape and size dynamics requires accounting for the particle internal degrees of freedom explicitly.

The dynamic two-scale model developed by Hütter et al. [11] presents a new class of models that provide insight about the degrees of freedom of permeable particles. The model accounts for the rate-dependent size change of the particles by treating the particle size as a separate degree of freedom. The developed model, however, focuses on spherical particles for which the particle geometry is described by its radius. Using this model, we have highlighted the effect of the size dynamics on the equilibrium properties [6], the flow properties [12], and the stress-relaxation behavior [13] of permeable-particle systems. This paper aims at generalizing the model developed by Hütter et al. [11] towards non-spherical particles. This requires modeling the particle shape explicitly, which naturally includes both the size and shape dynamics.

An essential step in the model development is the suitable choice of a variable that describes the particle shape. Several morphology measures have been introduced in the past, particularly in the field of mixing of immiscible fluids. The interfacial tensor in the Doi–Ohta model [14,15] provides an average description of the morphology of the entire dispersed phase in emulsions and immiscible polymer blends. In the present paper, a tensor is used for each individual particle, due to our interest in a many-particle description, as described in the following. For concentrated permeable-particle suspensions, tracking the exact particle surface can be computationally expensive. Therefore, we consider particles of ellipsoidal shape for simplicity. Ellipsoids cover a wide va-

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riety of shapes, ranging from platelets to spheres to threads [16,17]. Ellipsoidal droplet shapes are commonly used as an approximation of the microstructure of fluid blends. In fluid mixtures, this coarse-grained description depicts the local features of the microstructure, such as the size, shape, and orientation. An ellipsoid centered at the origin of the coordinate system is described by a second-rank tensor whose eigenvalues are the square of the (inverse) semi-axes lengths of the ellipsoid and whose eigenvectors give the direction of the principal axes of the ellipsoid. In general, the surface of an ellipsoid at a position $\boldsymbol{Q}$ of the coordinate system and whose axes are not necessarily aligned with the coordinate system is described by $(\boldsymbol{r}-\boldsymbol{Q})\cdot\boldsymbol{S}\cdot(\boldsymbol{r}-\boldsymbol{Q})=1$, with positive definite tensor $\boldsymbol{S}$. Several efforts have been dedicated to developing models describing the evolution of such tensors in response to deformation fields. For instance, the Maffettone and Minale (MM) model [18] describes the dynamics of ellipsoid droplets in a general flow field, based on a phenomenological description of the driving force and the relaxation mechanism. It has been shown experimentally and numerically how the internal morphology of a system affects its overall properties [19,20]. Rheology can be even a measure for probing the morphology [21]. Iza and Bousmina have highlighted the degree of complexity of the morphologies developed in a fluid-fluid mixture subjected to shear and upon cessation of flow [19]. This elucidates the importance of accurately and consistently describing the stress as a function of the microstructure. In order to achieve this, the evolution of the ellipsoidal tensor in affine deformation is used as the starting point. For purely affine deformation, each point in the ellipsoid is subjected to a velocity gradient $\boldsymbol{L}=(\nabla\boldsymbol{v})^{\mathrm{T}}$, where $\boldsymbol{v}$ is the applied flow field. Consequently, the evolution of the ellipsoid is given by $\dot{\boldsymbol{S}}=-\boldsymbol{L}^{\mathrm{T}}\cdot\boldsymbol{S}-\boldsymbol{S}\cdot\boldsymbol{L}$, which is a lower-convected time derivative [17]. The evolution of the ellipsoid in affine deformation can be equivalently described in terms of the inverse tensor $\boldsymbol{T}=\boldsymbol{S}^{-1}$. The evolution of $\boldsymbol{T}$ is upper-convected, that is $\dot{\boldsymbol{T}}=\boldsymbol{L}\cdot\boldsymbol{T}+\boldsymbol{T}\cdot\boldsymbol{L}^{\mathrm{T}}$ [17]. While the evolution of the particle-related ellipsoidal tensors in this paper is upper convected in nature, the interfacial tensor in the Doi–Ohta model [14,15] has lower-convected characteristics.

In this work, the dynamic two-scale model developed by Hütter et al. [11] for permeable particles is extended to also account for the mechanics and dynamics of the particle shape. Each particle is described with an ellipsoidal tensor. Non-equilibrium thermodynamics, namely the general equation for the non-equilibrium reversible-irreversible coupling (GENERIC) [22–24], is used to ensure that the developed model is thermodynamically consistent. The developed model is expressed in the form of stochastic differential equations, that are suitable for particle-based simulations, i.e. Brownian dynamics simulations.

This paper is organized as follows. In Section 2, the weak formulation of GENERIC is briefly described. This is used in Section 3 to develop a dynamic two-scale model for permeable particles that undergo shape and size changes. In Section 4, the model is presented in a form suitable for particle-based simulations. In Section 5, the model is split into purely-size and purely-shape dynamics, and applied to the case of non-interacting ellipsoidal particles. Finally, the paper is concluded with a discussion in Section 6.

2. Methods: Weak formulation of GENERIC

The general equation for the non-equilibrium reversible-irreversible coupling (GENERIC) [22–24] is exploited in this paper in order to develop a model that mutually couples mesoscopic degrees of freedom to macroscopic ones in a consistent manner. In this work, the weak formulation of GENERIC formulated in [11,25] is used, summarized in the following. For a closed system, the weak formulation of GENERIC [11,25] imposes the following conditions on the reversible (rev) and irreversible (irr) contributions to the time evolution of the energy E and the entropy S, respectively,

$$\dot{E}|_{\mathrm{rev}}=0, \tag{1a}$$

$$\dot{S}|_{\mathrm{rev}}=0, \tag{1b}$$

$$\dot{E}|_{\mathrm{irr}}=0, \tag{1c}$$

$$\dot{S}|_{\mathrm{irr}}\geq 0. \tag{1d}$$

The conditions (1) depict the following features of the system. On the one hand, the energy and entropy remain unaffected by the reversible dynamics, which is captured by (1a) and (1b), respectively. On the other hand, the irreversible dynamics does not affect the total energy and leads to non-negative entropy changes, as given by (1c) and (1d), respectively. It is noteworthy that, although the weak formulation of GENERIC (1) is less restrictive than its full formulation, it retains many of the essential features. Particularly, the degeneracy conditions in the full GENERIC formulation are reflected in conditions (1b) and (1c).

Using the chain rule, conditions (1) have implications on the evolution of the system variables $\boldsymbol{x}$. The chain rule for a general functional A is given by

$$\dot{A}[\boldsymbol{x}]=\sum_I\int\frac{\delta A}{\delta x_I(\boldsymbol{z})}\,\partial_t x_I(\boldsymbol{z})\,d\boldsymbol{z}, \tag{2}$$

where $\delta A/\delta x_I$ is a functional derivative of A with respect to x_I, $\boldsymbol{z}$ is the integration variable, and the summation runs over all variables in $\boldsymbol{x}$.

In the following, the conditions on the energy and entropy, (1), are used to develop a model for systems of permeable particles. This is achieved by, first choosing a sufficient set of variables describing the system, and second specifying the functionals of energy and entropy in terms of the chosen variables.

3. Model development

Similar to the model developed earlier in [11], a two-scale model is developed in this work, where both scales are mutually coupled. For instance, a deformation applied on the macroscopic level distorts the microstructure, this results in unbalanced interactions between the particles, which in turn give rise to macroscopic stresses. In this section, we derive a model that consistently couples both scales, particularly by providing a constitutive relation for the stress in terms of mesoscopic variables.

3.1. Choice of variables

For the two-scale model described for spherical particles [11], the macroscopic level, i.e. the solvent-particle system, is treated as a non-isothermal fluid. The macroscopic variables are, hence, the mass density $\rho(\boldsymbol{r})$, the momentum density $\boldsymbol{u}(\boldsymbol{r})=\boldsymbol{v}(\boldsymbol{r})/\rho$, where $\boldsymbol{v}$ is the macroscopic velocity field, and the temperature field $\vartheta(\boldsymbol{r})$. In all these variables, $\boldsymbol{r}$ is the macroscopic position. On the mesoscopic level, overdamped particle dynamics is considered. That is the particle velocities relax to the equilibrium distribution much faster than the time required for the applied deformation to cause a significant change in velocity. The reader is referred to [11] for more detail. Mesoscopically, each particle i is, hence, described with the position of its center $\boldsymbol{Q}_i$ measured relative to $\boldsymbol{r}$, and also by a tensor that captures the shape of the particle $\boldsymbol{T}_i$. The latter is introduced in place of the particle radius in [11], in order to describe the shape and size of the particle.

For practical reasons, a distribution function p of the mesoscopic states of all particle positions $\{\boldsymbol{Q}_i\}_{i=1,\dots,N}$ and shape tensors $\{\boldsymbol{T}_i\}_{i=1,\dots,N}$ is used a dynamic variable for the mesoscopic level of description. To account for inhomogeneous situations, the distribution function is made dependent on the macroscopic position, leading to $p=p(\boldsymbol{r},\{\boldsymbol{Q}_i\},\{\boldsymbol{T}_i\})$, where $\{\dots\}$ denotes the collection of variables for all particles, i.e. including all terms from $i=1$ until $i=N$. Averages over mesoscopic states, denoted by $\langle\cdot\rangle$, can be conveniently described in terms of p as

$$\langle h\rangle(\boldsymbol{r}) = n(\boldsymbol{r})^{-1}\int h\left(\boldsymbol{r},\{\boldsymbol{Q}_i\},\{\boldsymbol{T}_i\}\right)p\left(\boldsymbol{r},\{\boldsymbol{Q}_i\},\{\boldsymbol{T}_i\}\right)\,d\boldsymbol{Q}d\boldsymbol{T}, \tag{3}$$

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