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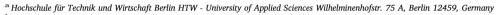
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Constitutive Theory of fiber suspensions

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ABSTRACT

We will demonstrate, that in fiber suspensions the stress tensor has a skew-symmetric part, i.e. fiber suspensions are micropolar fluids with non-zero couple stresses. Consequently, a continuum mechanical description of fiber suspensions requires the consideration of the balance of angular momentum in addition to the balance equations of mass, momentum and energy. An antisymmetric stress tensor is found for an isotropic orientation distribution of deformable fibers as well as for an anisotropic distribution of fiber orientations.

Mainly, the method of classical Thermodynamics of Irreversible Processes with internal variables is applied. The internal variables are fiber deformation variables and an orientation tensor in the case of a non-isotropic distribution of fiber orientations. In addition to the result on couple stresses, relaxation equations for the bend and twist deformation variables are derived.

Finally a mesoscopic background theory is discussed. In this approach a distribution of different fiber orientations and fiber deformations is assumed. The fiber orientation and deformation are additional variables in the domain of field quantities. The usual macroscopic fields of continuum mechanics are averages of mesoscopic fields over the different orientations and deformations. Macroscopic quantities characterizing the orientational order, the alignment tensors, and quantities characterizing fiber deformation, are defined by the help of the distribution function. They are internal variables in the macroscopic theory. The mesoscopic theory also demonstrates, that there is a skew symmetric part of the stress tensor in fiber suspensions.

1. Introduction

Fiber suspensions are interesting not only from the theoretical point of view, but they are very important as precursors of fiber composites. For instance, fiber reinforced concrete becomes more and more important in civil engineering, and the fresh concrete before hardening is a fiber suspension [1]. Another important example are glass or carbon fibers in polymer melts. In the melt, the fibers are reoriented during a flow process due to coupling between fiber orientation and velocity gradient [2–4]. The resulting fiber compounds are harder and stiffer than the pure polymer [5] and can be even electrically conducting in special cases. The constitutive properties depend on the fiber orientation distribution. Therefore, a constitutive model for the preceding polymer melt or fresh concrete with suspended fibers is important in order to predict the influences on the fiber orientation [6,7]. In addition to reorientation, the fibers may be deformed. The consequences of bend and twist deformation on the fiber suspension will be investigated here.

A phenomenological theory of suspensions and emulsions of weakly deformable spheres has been presented in [8]. The equations of motion for the particle deformation, and the constitutive equation for the stress

tensor have been derived in the whole range of concentrations of the emulsion. They are generalizations of earlier work on dilute suspensions [9–11] and emulsions [12,13]. Thermodynamic arguments have been applied in order to reduce the number of unknown constitutive coefficients. In semi-dilute suspensions hydrodynamic interactions between particles are important and their contribution to the stress tensor has been investigated. As it is expected for all materials with an internal structure the resulting stress tensor has an anti-symmetric part. An overview over calculations of the stress tensor of suspensions of elastic fibers of fixed orientation as well as on the stress tensor of rigid orientable fibers can be found in [14]. In contrast to these publications, we will consider both effects, fiber orientation and fiber deformation, simultaneously

Computer simulations of flexible fibers with interactions have been presented in [15–19]. Simulated suspensions exhibit heterogeneous structures, or flocculation, when the model fibers are flexible, have deformed equilibrium shapes, and interact through static friction forces. In another simulation [16] fibers undergo four different bending modes: stable U-shape, slight swing, violent flapping, and stable closure modes. However, the question of a skew-symmetric part of the stress

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tensor has not been investigated in these simulations. This is also the case in most of the literature on continuum mechanics of fiber suspensions: only the symmetric part of the stress tensor is considered (see f.i. [20–23]). The balance of angular momentum is not taken into account.

The derivation of constitutive equations on the ground of kinetic theory is similar for polymers (see f. i. [24]), which goes back to the Jeffery-model [25], and suspensions of fibers. An application of the stress tensor derived by Batchelor [26,27] from a kinetic background theory to corner flow of suspensions of orientable rigid rods can be found in [28]. The Jeffery-model has been generalized to a second gradient flow [29,30]. In this case rod bending is activated, and size-effects are predicted.

Finally the methods applied in the present paper, namely continuum mechanics with internal variables and Thermodynamics of Irreversible Processes has been applied successfully in other fields: liquid crystals [31], plasticity of metals and other solids [32], polymer solutions.

In the last section the methods of the so called mesoscopic theory are applied. This theory has been developed for liquid crystals [33–36]. For an overview over other possible applications see [37,38].

2. Irreversible thermodynamics of flexible fibers

The thermodynamic description of systems with dynamic (internal) variables has been applied with success to several kind of physical phenomena such as electric conduction [39] electric and magnetic polarization [40–42] heat conduction and radiation [43–48] viscoelastic and plastic deformations [49–62], liquid crystals [63]. The thermodynamic theory of visco-elasticity is based on dynamic variables which are second order symmetric tensors. They are related to the deformation of elastic micro-particles or to the distribution function of orientations of rod like or disk like rigid particles. For example some proteins, certain saccharoides, and liquid crystals are well approximated by the above model, but it fails, if particles are like elastic slender bars, e.g., in the case of fiber suspensions, in which the particles may be twisted and bent; their affine deformation is not relevant.

In the first part the flow induced anisotropy is neglected, and the orientation distribution of the fibers is presumed isotropic. The purpose here is to investigate the consequences of the flexibility of the particles. The deformation of a particle (bend and twist) stores energy, so influencing the macroscopic mechanical properties of the fluid. In the next section, the influence of an anisotropic orientation distribution of fibers is discussed.

In the following we will denote by the symbol : the contraction of second order tensors over all indices, in components: $\mathbf{A} \colon \mathbf{B} = A_{ik}B_{ki}$. The scalar product between vectors \boldsymbol{a} and \boldsymbol{b} is denoted by $\boldsymbol{a} \cdot \boldsymbol{b}$.

2.1. Deformation of a fiber

In our model the fibers are assumed to be straight if not loaded. Then one can chose a coordinate s along this fiber orientation and an orthogonal tensor U(s) describing the distortion of the fiber. The macroscopic angular distortion tensor defined by

$$\varphi : = U^T \cdot \frac{dU}{ds} \tag{2.1}$$

takes into account the local deformation of the flexible fibers, and is the average over all fiber orientations in the continuum element. s is the local coordinate along the fiber, and x is the position of the continuum element. s is only introduced in order to describe the local fiber deformation.

The tensor ϕ is obviously skew-symmetric as $\emph{\textbf{U}}$ is orthogonal,

$$\boldsymbol{U}^T \cdot \boldsymbol{U} = \boldsymbol{\delta},\tag{2.2}$$

where δ is the unit tensor and

$$\frac{dU^T}{ds} \cdot U + U^T \cdot \frac{dU}{ds} = 0, (2.3)$$

i.e.

$$\left(\boldsymbol{U}^{T} \cdot \frac{d\boldsymbol{U}}{ds}\right)^{T} + \boldsymbol{U}^{T} \cdot \frac{d\boldsymbol{U}}{ds} = 0.$$
(2.4)

This way, we introduce the angular distortion vector (the vector invariant of the angular distortion tensor) as

$$\overrightarrow{\varphi} \times \delta = \varphi. \tag{2.5}$$

Only in this case we will denote the vector by the symbol \rightarrow in order to distinguish it from the tensor φ .

Let $\mathbf n$ denote the unit vector tangential to the undeformed fiber. The scalar product of $\overrightarrow{\varphi}$ and $\mathbf n$ gives the twist:

$$t = \overrightarrow{\varphi} \cdot \mathbf{n},\tag{2.6}$$

and the component of $\overrightarrow{\varphi}$ perpendicular to **n** is the bend:

$$\mathbf{b} = \overrightarrow{\varphi} - \mathbf{n}(\mathbf{n} \cdot \overrightarrow{\varphi}) \tag{2.7}$$

An illustrating example will be shown.

As the fibers are elastic, two material coefficients, torsion stiffness μ_t and bending stiffness μ_b have to be introduced. The torque acting in a cross section of the fiber is given by

$$\tau = \mu_t \mathbf{n}(\mathbf{n} \cdot \overrightarrow{\varphi}) + \mu_b [\overrightarrow{\varphi} - \mathbf{n}(\mathbf{n} \cdot \overrightarrow{\varphi})]$$
 (2.8)

The elastic energy stored per unit length of a fiber is given by

$$u_e = \frac{\mu_t}{2} (\overrightarrow{\varphi} \cdot \mathbf{n})^2 + \frac{\mu_b}{2} (\overrightarrow{\varphi}^2 - (\overrightarrow{\varphi} \cdot \mathbf{n})^2). \tag{2.9}$$

The fibers are deformed by flow and they continuously relax. The angular distortion of an individual fiber $\overrightarrow{\varphi}$ depends on the local orientation of the fiber,

$$\vec{\varphi} = \vec{\varphi}(\mathbf{n}). \tag{2.10}$$

The function is odd, $\overrightarrow{\varphi}(-\mathbf{n}) = -\overrightarrow{\varphi}(\mathbf{n})$, according to the definition of $\overrightarrow{\varphi}$ Eq. (2.1), as turning the fiber (changing $\overrightarrow{\varphi}(\mathbf{n})$ to $\overrightarrow{\varphi}(-\mathbf{n})$) gives a - sign in the line element ds.

An obvious approximation for the function $\vec{\varphi}$ (**n**) is the first term of its expansion by spherical harmonics;

$$\overrightarrow{\varphi}(\mathbf{n}) = \alpha \cdot \mathbf{n},\tag{2.11}$$

where α is a second order pseudo tensor as $\overrightarrow{\varphi}$ is an axial vector. VERHAS [64] elaborated the theory based on this linear approximation and the theory gives only one relaxation time, while the relaxation times for twist and bend are expected to differ. As it will be shown in this section, the above shortcoming is ceased if the approximation (2.11) is improved with a third order term (with a traceless tensor β):

$$\overrightarrow{\varphi}(\mathbf{n}) = \alpha \cdot \mathbf{n} + \mathbf{n}(\mathbf{n} \cdot \boldsymbol{\beta} \cdot \mathbf{n}), \tag{2.12}$$

which can be decomposed as

$$\overrightarrow{\varphi}(\mathbf{n}) = \alpha_0 \mathbf{n} + \alpha^d \cdot \mathbf{n} + \alpha^d \cdot \mathbf{n} - \mathbf{n}(\mathbf{n} \cdot \alpha^d \cdot \mathbf{n}) + \mathbf{n}(\mathbf{n} \cdot T \cdot \mathbf{n}), \tag{2.13}$$

where $\alpha_0 = 1/3tr\alpha$, α^a is the skew symmetric part of α , α^d is the deviatoric part of α and T is the deviatoric part of the sum of the tensors α and β . The latter form shows the twist and bend separately; the first and the last term are due to twist, while the others are due to bend.

Inserting the approximation Eq. (2.12), the elastic energy of a fiber per unit fiber length reads

$$u_{e}(\mathbf{n}) = \frac{\mu_{t}}{2} (\alpha_{0} + \mathbf{n} \cdot \mathbf{T} \cdot \mathbf{n})^{2} + \frac{\mu_{b}}{2} (\alpha^{a} \cdot \mathbf{n} + \alpha^{d} \cdot \mathbf{n} - \mathbf{n} (\mathbf{n} \cdot \alpha^{d} \cdot \mathbf{n}))^{2},$$
(2.14)

the average of which over all possible fiber orientations is

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