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THERMODYNAMIC RESTRICTIONS ON CONSTITUTIVE FUNCTIONS FOR FIBER SUSPENSIONS

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ABSTRACT. The constitutive properties of fiber suspensions are investigated with the methods of thermodynamics. Fiber orientation, orientation change velocity and gradient of orientation are considered as relevant variables for the constitutive functions, and the Second Law of Thermodynamics in the form of the dissipation inequality is exploited by a method introduced by I-S. Liu [Arch. Rat. Mech. Analysis **46**, 131 (1972)]. The restrictions on the constitutive functions show, that the fiber suspension is a micropolar continuum with non-vanishing couple stresses. In addition it is shown that the classical relation of entropy flux being heat flux over temperature holds only in the special case that the free energy density does not depend on the orientation change velocity, otherwise there exists an extra entropy flux.

1. Introduction

Fiber suspensions are important in many fields of application, f.i. as precursors of fiber reinforced polymers or fiber reinforced concrete. A prediction of flow induced orientation and deformation of fibers is interesting, also from a practical point of view, because the mechanical and other properties of the resulting fiber composites depend on fiber orientation and deformation during the production process. A continuum mechanical model of the interaction of the flow field with fiber orientations have been presented by Folgar and Tucker (1984), Advani and Tucker (1987), Byron Bird *et al.* (1987), Tucker and Advani (1994), and Azaiez (1996), but there the fibers have been assumed to be rigid. Fiber suspensions of rigid fibers with an orientational order have an analogy to liquid crystals. In case of liquid crystals an orientational order (an anisotropic orientation distribution) leads to an antisymmetric part of the stress tensor, and the liquid crystal is a micropolar medium (Eringen 1978). Fiber suspensions of flexible fibers with orientational order have been considered by Papenfuss and Verhás (2018) with the methods of Thermodynamics of Irreversible Processes with internal variables.

Our aim here is to show, that a suspension of flexible fibers is a micropolar continuum, even if the fiber orientations are isotropic (no orientational order). Consequently, in continuum mechanics of fiber suspensions the balance of angular momentum has to be taken into account in addition to the balance equations of mass, momentum and energy.

The method applied here to derive the restrictions on constitutive functions for fiber suspensions is the method introduced by Liu (1972). From a very basic amendment to the second law of thermodynamics, on physical arguments one can show that the requirement of a positive entropy production density (the Second Law of Thermodynamics) restricts possible constitutive functions and does *not* rule out certain process directions in non-equilibrium (Muschik and Ehrentraut 1996). The most general way to derive these restrictions on constitutive functions is the method by Liu (1972).

2. Balance equations and the Second Law of Thermodynamics

The governing balance equations for the fields of mass density ρ, material velocity of the fluid-fiber mixture $\boldsymbol{v}$, specific internal angular momentum $\boldsymbol{s}$, and specific internal energy u are listed below.

Mass:

$$\frac{d\rho}{dt} + \rho \nabla \cdot \boldsymbol{v} = 0 \ , \tag{2.1}$$

where the derivative $\frac{d}{dt}$ is the material (or total) time derivative:

$$\frac{d}{dt} = \frac{\partial}{\partial t} + (\boldsymbol{v} \cdot \nabla) \, . \tag{2.2}$$

Linear momentum:

$$\rho \frac{d\boldsymbol{v}}{dt} = \rho \boldsymbol{f} + \nabla \cdot \boldsymbol{t}, \tag{2.3}$$

where $\boldsymbol{t}$ is Cauchy's stress tensor and $\boldsymbol{f}$ is the body force per unit mass; the definition for the divergence used here reads in Cartesian components:

$$(\nabla \cdot \boldsymbol{t})_i = \nabla_j t_{ij} \, . \tag{2.4}$$

Angular momentum:

$$\rho \frac{d\boldsymbol{s}}{dt} = 2\boldsymbol{w}(\boldsymbol{t}) + \rho \boldsymbol{m} + \nabla \cdot \boldsymbol{\Pi}, \tag{2.5}$$

where $\boldsymbol{m}$ is the torque exerted on the material by external fields and $\boldsymbol{\Pi}$ is the couple stress tensor; the vector $\boldsymbol{w}(\boldsymbol{t})$ stands for the vector invariant of the antisymmetric part of Cauchy's stress tensor, which is zero in case of a symmetric stress tensor.

Internal energy:

$$\rho \frac{du}{dt} + \nabla \cdot \boldsymbol{q} = \nabla \boldsymbol{v} : \boldsymbol{t} + \boldsymbol{\Pi} : \nabla \boldsymbol{\omega} \, , \tag{2.6}$$

where $\nabla \boldsymbol{v}$ is the velocity gradient, $\boldsymbol{q}$ is the heat flux and $\boldsymbol{\omega}$ is the angular velocity of the fibers in the volume element; it is reasonable to assume that the fibers are co-rotating with the volume element, *i.e.*,

$$\boldsymbol{\omega} = \nabla \times \boldsymbol{v} \, . \tag{2.7}$$

This is a classical result of Doi and Edwards (1986), and it has been shown by Abisset-Chavanne *et al.* (2015) that the angular velocity of a flexible fiber is equal to the vorticity of the flow field, even in a second gradient theory.

In addition, we have the balance of entropy:

$$\rho \frac{d\eta}{dt} + \nabla \cdot \boldsymbol{\phi} = \sigma \geq 0, \tag{2.8}$$

where the inequality is the local formulation of the Second Law of Thermodynamics. Entropy supply has been neglected, as well as energy supply (radiation) in the balance of internal energy.

3. Choice of the state space

The system of balance equations is under-determined, as as long as no constitutive equations are specified for the constitutive quantities of stress tensor $\boldsymbol{t}$, torque density $\boldsymbol{m}$, couple stresses Π, heat flux $\boldsymbol{q}$, specific entropy η and entropy flux $\boldsymbol{\phi}$. The domain of the constitutive functions is denoted as state space.

The restrictions on the constitutive functions follow after this set of variables for material properties has been chosen. The restrictions do not completely determine the material behavior, as it is natural, because there exist different materials with the same set of variables, but different constitutive properties. The results of the exploitation of the dissipation inequality give the most general framework compatible with the second law of thermodynamics.

In the example of fiber suspensions it is reasonable to assume that fiber orientation plays a role for the constitutive behavior. The local fiber orientation is described by an orthogonal second order tensor $\boldsymbol{Q}$. $\boldsymbol{Q}$ is the mapping (the rotation) between the orientation vector of the (undistorted) fiber and a reference coordinate system. With the tensor Q it would also be possible to account for the orientation of biaxial elements, such as plates, but this is out of scope of the present paper.

Two cases may be considered in an analogous way: In the example of short fibers, deformation of the fibers does not play a role, but the fiber orientation may vary with position. For long fibers (much longer than the size of the continuum element) deformation becomes important. In this case, $\boldsymbol{Q}$ is the orientation of a fiber segment. If the fiber is not straight, but deformed, $\boldsymbol{Q}$ varies with position. Both cases may be treated by a second order tensor $\boldsymbol{O}$ for the local gradient or deformation of the fibers, respectively. $\boldsymbol{O}$ is defined as

$$\boldsymbol{O} = \frac{1}{2}\left((\nabla \boldsymbol{Q}^T) \cdot \boldsymbol{Q}\right) : \boldsymbol{\epsilon} \tag{3.9}$$

with the totally antisymmetric third order tensor $\boldsymbol{\epsilon}$. We also include the time derivative Ω of the fiber orientation:

$$\frac{\partial \boldsymbol{Q}}{\partial t} = \boldsymbol{\Omega} \times \boldsymbol{Q} \tag{3.10}$$

in the set of relevant variables for constitutive functions.

The constitutive mappings are defined on the following domain:

$$Z = \{\rho, T, \nabla \boldsymbol{v}, \boldsymbol{Q}, \boldsymbol{O}, \boldsymbol{\Omega}\},, \tag{3.11}$$

with temperature T. All constitutive quantities do not depend on $\boldsymbol{v}$, but $\boldsymbol{v}$ is included in the set of variables, because the gradient of $\boldsymbol{v}$ is relevant. Acceleration $\dot{\boldsymbol{v}}$ again is not in the domain of constitutive functions, but is a higher derivative. Apart from the equilibrium variables mass density and temperature it includes the velocity gradient and the fiber orientation related variables.

4. Exploitation of the dissipation inequality according to Liu

As the materials discussed here are micropolar media we will take into account the balance of internal angular momentum in addition to the balances of mass, momentum, and energy. The following inequality has to be exploited:

$$
\begin{aligned}
\rho \frac{d\eta}{dt} + \nabla\cdot\boldsymbol{\phi} + \lambda^{\rho}\left(\frac{d\rho}{dt} + \rho\nabla\cdot\boldsymbol{v}\right) \\
+\boldsymbol{\lambda}^{p}\cdot\left(\rho\frac{d\boldsymbol{v}}{dt} - \nabla\cdot\boldsymbol{t} - \rho\boldsymbol{f}\right) \\
+\lambda^{u}\left(\rho\frac{du}{dt} + \nabla\cdot\boldsymbol{q} - \boldsymbol{t}:\nabla\boldsymbol{v} + \boldsymbol{\Pi}:\nabla\boldsymbol{\Omega}\right) \\
+\boldsymbol{\lambda}^{s}\cdot\left(\rho\frac{d\boldsymbol{s}}{dt} - \boldsymbol{\epsilon}:\boldsymbol{t} + \nabla\cdot\boldsymbol{\Pi} + \rho\boldsymbol{m}\right) \geq 0 .
\end{aligned}
\tag{4.12}
$$

After exploiting the differentiations of the constitutive functions, defined on the state space (3.11), according to the chain rule it results an inequality linear in the following higher derivatives:

$$
\dot{T}, \dot{\rho}, \dot{\boldsymbol{v}}, \frac{d(\nabla\boldsymbol{v})}{dt}, \dot{\boldsymbol{O}}, \dot{\boldsymbol{\Omega}}, \nabla\rho, \nabla T, \nabla\nabla\boldsymbol{v}, \nabla\boldsymbol{O}, \nabla\Omega . \tag{4.13}
$$

These higher derivatives are not all independent, but one constraint between them has to be taken into account. To show this we will use components with respect to a Cartesian coordinate system.

Proposition:

$$
\frac{d\boldsymbol{O}}{dt} = (\nabla\boldsymbol{\Omega})^{T} + \frac{1}{2}\left(\boldsymbol{\epsilon}\cdot\boldsymbol{Q}:\frac{\partial\boldsymbol{Q}^{T}}{\partial\boldsymbol{x}}\right)\cdot\frac{\partial\boldsymbol{v}}{\partial\boldsymbol{x}} , \tag{4.14}
$$

or, in components:

$$
\frac{dO_{ik}}{dt} = \frac{\partial\Omega_i}{\partial x_k} + \frac{1}{2}\varepsilon_{irl}Q_{ls}\frac{\partial Q_{rs}}{\partial x_m}\frac{\partial v_m}{\partial x_k} . \tag{4.15}
$$

The proof of this proposition is shown in the appendix. $\boldsymbol{Q}$, $\nabla\boldsymbol{v}$ and $\nabla\boldsymbol{Q}$ are state space variables, whereas $\nabla\boldsymbol{\Omega}$ is not included in the state space. This gradient shows up in the list of higher derivatives.

After inserting this constraint we can write down the Liu-equations, corresponding to the different higher derivatives:

$$\dot{\rho}: \quad \rho\frac{\partial \eta}{\partial \rho} + \lambda^u \rho \frac{\partial u}{\partial \rho} + \lambda^\rho + \rho \boldsymbol{\lambda}^s \cdot \frac{\partial \boldsymbol{s}}{\partial \rho} = 0 \quad (4.16)$$

$$\dot{T}: \quad \rho\frac{\partial \eta}{\partial T} + \lambda^u \rho \frac{\partial u}{\partial T} + \rho \boldsymbol{\lambda}^s \cdot \frac{\partial \boldsymbol{s}}{\partial T} = 0 \quad (4.17)$$

$$\dot{\nabla \boldsymbol{v}}: \quad \rho\frac{\partial \eta}{\partial \nabla \boldsymbol{v}} + \lambda^u \rho \frac{\partial u}{\partial \nabla \boldsymbol{v}} + \rho \boldsymbol{\lambda}^s \cdot \frac{\partial \boldsymbol{s}}{\partial \nabla \boldsymbol{v}} = 0 \quad (4.18)$$

$$\nabla \boldsymbol{\Omega}: \quad \rho\frac{\partial \eta}{\partial \boldsymbol{O}} + \frac{\partial \boldsymbol{\Phi}}{\partial \boldsymbol{\Omega}} - \boldsymbol{\lambda}^p \cdot \frac{\partial \boldsymbol{t}}{\partial \boldsymbol{\Omega}} + \boldsymbol{\lambda}^s \cdot \left(\rho \frac{\partial \boldsymbol{s}}{\partial \boldsymbol{O}} - \frac{\partial \boldsymbol{\Pi}}{\partial \boldsymbol{\Omega}}\right) + \lambda^u \left(-\boldsymbol{\Pi} + \frac{\partial \boldsymbol{q}}{\partial \boldsymbol{\Omega}}\right) = 0 \quad (4.19)$$

$$\dot{\boldsymbol{\Omega}}: \quad \rho\frac{\partial \eta}{\partial \boldsymbol{\Omega}} + \lambda^u \frac{\partial u}{\partial \boldsymbol{\Omega}} + \rho \boldsymbol{\lambda}^s \cdot \frac{\partial \boldsymbol{s}}{\partial \boldsymbol{\Omega}} = 0 \quad (4.20)$$

$$\nabla \rho: \quad \frac{\partial \boldsymbol{\Phi}}{\partial \rho} - \boldsymbol{\lambda}^p \cdot \frac{\partial \boldsymbol{t}}{\partial \rho} - \boldsymbol{\lambda}^s \cdot \frac{\partial \boldsymbol{\Pi}}{\partial \rho} + \lambda^u \frac{\partial \boldsymbol{q}}{\partial \rho} = 0 \quad (4.21)$$

$$\nabla T: \quad \frac{\partial \boldsymbol{\Phi}}{\partial T} - \boldsymbol{\lambda}^p \cdot \frac{\partial \boldsymbol{t}}{\partial T} - \boldsymbol{\lambda}^s \cdot \frac{\partial \boldsymbol{\Pi}}{\partial T} + \lambda^u \frac{\partial \boldsymbol{q}}{\partial T} = 0 \quad (4.22)$$

$$\nabla \nabla \boldsymbol{v}: \quad \frac{\partial \boldsymbol{\Phi}}{\partial \nabla \boldsymbol{v}} - \boldsymbol{\lambda}^p \cdot \frac{\partial \boldsymbol{t}}{\partial \nabla \boldsymbol{v}} - \boldsymbol{\lambda}^s \cdot \frac{\partial \boldsymbol{\Pi}}{\partial \nabla \boldsymbol{v}} + \lambda^u \frac{\partial \boldsymbol{q}}{\partial \nabla \boldsymbol{v}} = 0 \quad (4.23)$$

$$\nabla \boldsymbol{O}: \quad \frac{\partial \boldsymbol{\Phi}}{\partial \boldsymbol{O}} - \boldsymbol{\lambda}^p \cdot \frac{\partial \boldsymbol{t}}{\partial \boldsymbol{O}} - \boldsymbol{\lambda}^s \cdot \frac{\partial \boldsymbol{\Pi}}{\partial \boldsymbol{O}} + \lambda^u \frac{\partial \boldsymbol{q}}{\partial \boldsymbol{O}} = 0 \quad (4.24)$$

$$\frac{d\boldsymbol{v}}{dt}: \quad \rho \boldsymbol{\lambda}^p = 0 \quad (4.25)$$

From this set of equations the multipliers λ^ρ, $\boldsymbol{\lambda}^p$, $\boldsymbol{\lambda}^s$, and λ^u can be calculated. Between the specific spin density and the orientation change velocity $\boldsymbol{\Omega}$ the relation

$$\boldsymbol{s} = \boldsymbol{\Theta} \cdot \boldsymbol{\Omega} \quad (4.26)$$

holds, where $\boldsymbol{\Theta}$ is the moment of inertia tensor, which is assumed to be constant. In case of suspensions of flexible fibers this is only an approximation, because in principle this tensor changes if the fibers are deformed. We assume here that these deformations are small and the variation of $\boldsymbol{\Theta}$ can be neglected. Then the specific spin density $\boldsymbol{s}$ depends only on the orientation change velocity $\boldsymbol{\Omega}$, and all other partial derivatives vanish. In this case we have

$$\frac{\partial \boldsymbol{s}}{\partial \boldsymbol{\Omega}} = \boldsymbol{\Theta} \quad (4.27)$$

and the equations for the multipliers simplify to

$$\lambda^u = -\frac{\frac{\partial \eta}{\partial T}}{\frac{\partial u}{\partial T}} = -\frac{1}{T} \quad (4.28)$$

$$\lambda^\rho = -\rho \frac{\partial \eta}{\partial \rho} + \frac{1}{T} \rho \frac{\partial u}{\partial \rho} \quad (4.29)$$

$$\boldsymbol{\lambda}^s = -\frac{\partial \left(\eta - \frac{1}{T} u\right)}{\partial \boldsymbol{\Omega}} \cdot \boldsymbol{\Theta}^{-1} \quad (4.30)$$

$$\boldsymbol{\lambda}^p = 0, \quad (4.31)$$

where for the derivative $(\frac{\partial \eta}{\partial T})(\frac{\partial u}{\partial T})^{-1}$ we insert $\frac{1}{T}$. This relation is known in equilibrium. In non equilibrium it needs some additional argumentations, as illustrated by Müller (1985). The remaining equations (4.18), (4.19), (4.21), (4.22), (4.23), and (4.24) give, after inserting the multipliers, the restrictions on constitutive functions. This will be shown here only under the assumption of a constant moment of inertia tensor. We have:

$$\frac{\partial\left(\eta - \frac{1}{T}u\right)}{\partial \nabla \boldsymbol{v}} = 0 \tag{4.32}$$

$$\boldsymbol{\Pi} = -\frac{1}{T}\left(\rho \frac{\partial\left(\eta - \frac{1}{T}u\right)}{\partial \boldsymbol{O}} + \frac{\partial \boldsymbol{\Phi}}{\partial \boldsymbol{\Omega}} + \frac{\partial\left(\eta - \frac{1}{T}u\right)}{\partial \boldsymbol{\Omega}} \cdot \boldsymbol{\Theta}^{-1} \cdot \frac{\partial \boldsymbol{\Pi}}{\partial \boldsymbol{\Omega}}\right) \tag{4.33}$$

$$\frac{\partial \boldsymbol{\Phi}}{\partial \rho} - \frac{1}{T}\frac{\partial \boldsymbol{q}}{\partial \rho} = -\frac{\partial\left(\eta - \frac{1}{T}u\right)}{\partial \boldsymbol{\Omega}} \cdot \boldsymbol{\Theta}^{-1} \cdot \frac{\partial \boldsymbol{\Pi}}{\partial \rho} \tag{4.34}$$

$$\frac{\partial \boldsymbol{\Phi}}{\partial T} - \frac{1}{T}\frac{\partial \boldsymbol{q}}{\partial T} = -\frac{\partial\left(\eta - \frac{1}{T}u\right)}{\partial \boldsymbol{\Omega}} \cdot \boldsymbol{\Theta}^{-1} \cdot \frac{\partial \boldsymbol{\Pi}}{\partial T} \tag{4.35}$$

$$\frac{\partial \boldsymbol{\Phi}}{\partial \nabla \boldsymbol{v}} - \frac{1}{T}\frac{\partial \boldsymbol{q}}{\partial \nabla \boldsymbol{v}} = -\frac{\partial\left(\eta - \frac{1}{T}u\right)}{\partial \boldsymbol{\Omega}} \cdot \boldsymbol{\Theta}^{-1} \cdot \frac{\partial \boldsymbol{\Pi}}{\partial \nabla \boldsymbol{v}} \tag{4.36}$$

$$\frac{\partial \boldsymbol{\Phi}}{\partial \boldsymbol{O}} - \frac{1}{T}\frac{\partial \boldsymbol{q}}{\partial \boldsymbol{O}} = -\frac{\partial\left(\eta - \frac{1}{T}u\right)}{\partial \boldsymbol{\Omega}} \cdot \boldsymbol{\Theta}^{-1} \cdot \frac{\partial \boldsymbol{\Pi}}{\partial \boldsymbol{O}} \tag{4.37}$$

Introducing the free energy density $f := u - T\eta$ and the difference $\boldsymbol{k} = \boldsymbol{\Phi} - \frac{1}{T}\boldsymbol{q}$, the resulting restrictions on the constitutive functions can be written as:

$$\frac{\partial f}{\partial \nabla \boldsymbol{v}} = 0 \tag{4.38}$$

$$\boldsymbol{\Pi} = \frac{1}{T^2}\rho \frac{\partial f}{\partial \boldsymbol{O}} + \frac{1}{T}\frac{\partial \boldsymbol{\Phi}}{\partial \boldsymbol{\Omega}} - \frac{1}{T^2}\frac{\partial f}{\partial \boldsymbol{\Omega}} \cdot \boldsymbol{\Theta}^{-1} \cdot \frac{\partial \boldsymbol{\Pi}}{\partial \boldsymbol{\Omega}} \tag{4.39}$$

$$\frac{\partial \boldsymbol{k}}{\partial u_i} = \frac{1}{T}\frac{\partial f}{\partial \boldsymbol{\Omega}} \cdot \boldsymbol{\Theta}^{-1} \cdot \frac{\partial \boldsymbol{\Pi}}{\partial u_i}, \ \text{for}\, u_i \in \{\rho, T, \nabla \boldsymbol{v}, \boldsymbol{O}\} \tag{4.40}$$

Equation (4.40) shows that the difference $\boldsymbol{k} = \boldsymbol{\Phi} - \frac{1}{T}\boldsymbol{q}$ is surely non-zero, if the free energy density depends on the orientation change velocity ($\frac{\partial f}{\partial \boldsymbol{\Omega}} \neq 0$), and if the couple stresses $\boldsymbol{\Pi}$ depend on any of the variables ρ, T, $\nabla \boldsymbol{v}$, $\boldsymbol{O}$. In this case the very frequently made constitutive assumption (see for instance Irreversible Thermodynamics) of the entropy flux $\boldsymbol{\Phi}$ being heat flux divided by temperature is not fulfilled. Equation (4.39) is a differential equation for the couple stress. It reduces to an algebraic equation, if the free energy density and the entropy flux doe not depend on $\boldsymbol{\Omega}$. In this case the couple stresses can be calculated as a derivative of the free energy density

$$\boldsymbol{\Pi} = \frac{1}{T^2}\rho \frac{\partial f}{\partial \boldsymbol{O}}. \tag{4.41}$$

4.1. **The entropy production.** The residual inequality is built up by all terms in equation (4.12), which contain no higher derivatives, but only state space functions. The constraint equation (4.15) has been inserted. We will deal here only with the case of a constant moment of inertia tensor. For the multipliers equations (4.28) to (4.31) are inserted:

$$\begin{aligned}\sigma = {}&\rho \frac{\partial \eta}{\partial \boldsymbol{Q}} : \dot{\boldsymbol{Q}} - \frac{\rho}{2}\frac{\partial \eta}{\partial \boldsymbol{O}} \cdot \nabla \boldsymbol{v} \cdot (\nabla \boldsymbol{Q}) \cdot \boldsymbol{Q}^T \cdot : \boldsymbol{\epsilon} + \frac{\partial \boldsymbol{\Phi}}{\partial \boldsymbol{Q}} \cdot : \frac{\partial \boldsymbol{Q}}{\partial \boldsymbol{x}} \\ &+ \lambda^\rho \nabla \cdot \boldsymbol{v} - \boldsymbol{\lambda}^s \cdot \left(\frac{\partial \boldsymbol{\Pi}}{\partial \boldsymbol{Q}} \cdot : \frac{\partial \boldsymbol{Q}}{\partial \boldsymbol{x}} + \rho \boldsymbol{m} - \boldsymbol{\epsilon} : \boldsymbol{t} \right) \\ &+ \lambda^u \left(\rho \frac{\partial u}{\partial \boldsymbol{Q}} : \dot{\boldsymbol{Q}} - \frac{\rho}{2}\frac{\partial u}{\partial \boldsymbol{O}} \cdot \nabla \boldsymbol{v} \cdot (\nabla \boldsymbol{Q}) \cdot \boldsymbol{Q}^T \cdot : \boldsymbol{\epsilon} + (\boldsymbol{\epsilon} : \boldsymbol{t}) \cdot \boldsymbol{s} \right. \\ &\left. + \frac{\partial \boldsymbol{q}}{\partial \boldsymbol{Q}} \cdot : \frac{\partial \boldsymbol{Q}}{\partial \boldsymbol{x}} - \boldsymbol{t} : (\nabla \boldsymbol{v}) \right) \\ = {}&\rho \frac{\partial \eta}{\partial \boldsymbol{Q}} : \dot{\boldsymbol{Q}} - \frac{\rho}{2}\frac{\partial \eta}{\partial \boldsymbol{O}} \cdot \nabla \boldsymbol{v} \cdot (\nabla \boldsymbol{Q}) \cdot \boldsymbol{Q}^T \cdot : \boldsymbol{\epsilon} + \frac{\partial \boldsymbol{\Phi}}{\partial \boldsymbol{Q}} \cdot : \frac{\partial \boldsymbol{Q}}{\partial \boldsymbol{x}} \\ &+ \frac{1}{T}\rho \frac{\partial f}{\partial \rho} \nabla \cdot \boldsymbol{v} - \frac{1}{T}\frac{\partial f}{\partial \boldsymbol{\Omega}} \cdot \boldsymbol{\Theta}^{-1} \cdot \left(\frac{\partial \boldsymbol{\Pi}}{\partial \boldsymbol{Q}} \cdot : \frac{\partial \boldsymbol{Q}}{\partial \boldsymbol{x}} + \rho \boldsymbol{m} - \boldsymbol{\epsilon} : \boldsymbol{t} \right) \\ &- \frac{1}{T} \left(\rho \frac{\partial u}{\partial \boldsymbol{Q}} : \dot{\boldsymbol{Q}} - \frac{\rho}{2}\frac{\partial u}{\partial \boldsymbol{O}} \cdot \nabla \boldsymbol{v} \cdot (\nabla \boldsymbol{Q}) \cdot \boldsymbol{Q}^T \cdot : \boldsymbol{\epsilon} + (\boldsymbol{\epsilon} : \boldsymbol{t}) \cdot \boldsymbol{s} \right. \\ &\left. + \frac{\partial \boldsymbol{q}}{\partial \boldsymbol{Q}} \cdot : \frac{\partial \boldsymbol{Q}}{\partial \boldsymbol{x}} - \boldsymbol{t} : (\nabla \boldsymbol{v}) \right)\end{aligned}$$

$$\begin{aligned}\sigma = {}& \underbrace{-\frac{\rho}{T}\frac{\partial f}{\partial \boldsymbol{Q}} : \dot{\boldsymbol{Q}}}_{\text{change of orientational order}} \\ &+ \underbrace{\frac{\rho}{2T}\frac{\partial f}{\partial \boldsymbol{O}} \cdot \nabla \boldsymbol{v} \cdot (\nabla \boldsymbol{Q}) \cdot \boldsymbol{Q}^T \cdot : \boldsymbol{\epsilon}}_{\text{coupling between viscous flow and orientational order}} \\ &+ \underbrace{\frac{\partial \boldsymbol{k}}{\partial \boldsymbol{Q}} \cdot : \frac{\partial \boldsymbol{Q}}{\partial \boldsymbol{x}}}_{\text{transport of orientation}} \underbrace{+ \frac{1}{T}\left(\rho \frac{\partial f}{\partial \rho} + \frac{1}{3} trace(\boldsymbol{t}) \right) \nabla \cdot \boldsymbol{v}}_{\text{volume viscosity}} \\ &- \underbrace{\frac{1}{T}\frac{\partial f}{\partial \boldsymbol{\Omega}} \cdot \boldsymbol{\Theta}^{-1} \cdot \left(\frac{\partial \boldsymbol{\Pi}}{\partial \boldsymbol{Q}} \cdot : \frac{\partial \boldsymbol{Q}}{\partial \boldsymbol{x}} \right)}_{\text{coupling between change of orientation and gradient of orientation}} \\ & \underbrace{-\frac{1}{T}\frac{\partial f}{\partial \boldsymbol{\Omega}} \cdot \boldsymbol{\Theta}^{-1} \cdot (\rho \boldsymbol{m} - \boldsymbol{\epsilon} : \boldsymbol{t})}_{\text{rotational motion}} \\ & \underbrace{-\frac{1}{T}\left((\boldsymbol{\epsilon} : \boldsymbol{t}) \cdot \boldsymbol{s} - \boldsymbol{t}^{antisym} : (\nabla \boldsymbol{v}^{antisym}) \right)}_{\text{rotational viscosity}} - \underbrace{\frac{1}{T} \overline{\boldsymbol{t}} : \overline{\nabla \boldsymbol{v}}}_{\text{shear viscosity}} \geq 0 \qquad (4.42)\end{aligned}$$

with the symmetric traceless part $\overline{}$ of a second order tensor. The interpretation of the different terms is given in the equation. A term of the form $-\frac{1}{T^2}\boldsymbol{q} \cdot \nabla T$ does not occur here, because the temperature gradient was not included in the state space, but is a higher derivative, and the entropy production is a function of the state space variables. If there is a heat flux $\boldsymbol{q} \neq 0$, it is not caused by a temperature gradient in this example.

5. Conclusions

It could be shown that the assumption made f.i. in Thermodynamics of Irreversible Processes (TIP) concerning the entropy flux being heat flux divided by temperature does not contradict the results of the Liu-procedure, if the free energy density does not depend on the orientation change velocity of the fibers. In this case $\boldsymbol{k} = 0$ and $\boldsymbol{\Phi} = \frac{\boldsymbol{q}}{T}$. In classical TIP this assumption is fulfilled, because the free energy density depends on the equilibrium variables only. However, if the orientation change velocity is included in the set of variables, the entropy flux might be not simply heat flux divided by temperature, as a result of the exploitation of the dissipation inequality. This can be interpreted as non-convective entropy transport due to change of fiber orientations. Equation (4.41) shows, that the couple stresses do not vanish, because the free energy density depends on fiber deformation $\boldsymbol{O}$ (bend and twist of fibers increase the internal energy of the mixture). This shows clearly, that the fiber suspension is a micropolar medium. The stress tensor cannot be supposed to be symmetric, and the balance of angular momentum has to be taken into account.

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Appendix

Proof of the proposition on the time derivative of the state space variable *O*

Proposition:

$$\frac{d\boldsymbol{O}}{dt} = (\nabla\boldsymbol{\Omega})^T + \frac{1}{2}\left(\boldsymbol{\epsilon}\cdot\boldsymbol{Q} : \frac{\partial \boldsymbol{Q}^T}{\partial \boldsymbol{x}}\right)\cdot\frac{\partial \boldsymbol{v}}{\partial \boldsymbol{x}} \tag{5.43}$$

or, in components:

$$\frac{dO_{ik}}{dt} = \frac{\partial \Omega_i}{\partial x_k} + \frac{1}{2}\varepsilon_{irl}Q_{ls}\frac{\partial Q_{rs}}{\partial x_m}\frac{\partial v_m}{\partial x_k}. \tag{5.44}$$

Proof:

In components we have:

$$\begin{aligned}
\frac{dO_{ik}}{dt} = -\frac{1}{2}\varepsilon_{irl}\frac{d}{dt}\left(\frac{\partial Q_{rs}}{\partial x_k}Q_{ls}\right) = \\
-\frac{1}{2}\varepsilon_{irl}\left(\frac{d}{dt}\left(\frac{\partial Q_{rs}}{\partial x_k}\right)Q_{ls} + \frac{\partial Q_{rs}}{\partial x_k}\frac{dQ_{ls}}{dt}\right) = \\
-\frac{1}{2}\varepsilon_{irl}\left(\left(\frac{\partial}{\partial t} + v_m\frac{\partial}{\partial x_m}\right)\left(\frac{\partial Q_{rs}}{\partial x_k}\right)Q_{ls} + \frac{\partial Q_{rs}}{\partial x_k}\varepsilon_{lkm}\Omega_k Q_{ms}\right) = \\
-\frac{1}{2}\varepsilon_{irl}\left(\left(\frac{\partial}{\partial x_k}\left(\frac{\partial Q_{rs}}{\partial t} + v_m\frac{\partial Q_{rs}}{\partial x_m}\right) - \frac{\partial v_m}{\partial x_k}\frac{\partial Q_{rs}}{\partial x_m}\right)Q_{ls} + \frac{\partial Q_{rs}}{\partial x_k}\varepsilon_{lkm}\Omega_k Q_{ms}\right) = \\
-\frac{1}{2}\varepsilon_{irl}\left(\left(\frac{\partial}{\partial x_k}\frac{dQ_{rs}}{dt} - \frac{\partial v_m}{\partial x_k}\frac{\partial Q_{rs}}{\partial x_m}\right)Q_{ls} + \frac{\partial Q_{rs}}{\partial x_k}\varepsilon_{lkm}\Omega_k Q_{ms}\right) = \\
-\frac{1}{2}\varepsilon_{irl}\left(\left(\frac{\partial}{\partial x_k}\left(\varepsilon_{rop}\Omega_o Q_{ps}\right) - \frac{\partial v_m}{\partial x_k}\frac{\partial Q_{rs}}{\partial x_m}\right)Q_{ls} + \frac{\partial Q_{rs}}{\partial x_k}\varepsilon_{lkm}\Omega_k Q_{ms}\right) = \\
\frac{1}{2}\left(\left(\delta_{io}\delta_{lp} - \delta_{ip}\delta_{lo}\right)\left(\frac{\partial \Omega_o}{\partial x_k}Q_{ps} + \Omega_o\frac{\partial Q_{ps}}{\partial x_k}\right) + \frac{1}{2}\varepsilon_{irl}\frac{\partial v_m}{\partial x_k}\frac{\partial Q_{rs}}{\partial x_m}\right)Q_{ls} - \\
\frac{1}{2}\left(\delta_{ik}\delta_{rm} - \delta_{im}\delta_{rk}\right)\frac{\partial Q_{rs}}{\partial x_k}\Omega_k Q_{ms} = \\
\frac{1}{2}\left(\frac{\partial \Omega_i}{\partial x_k}Q_{ls}Q_{ls} - \frac{\partial \Omega_l}{\partial x_k}Q_{is}Q_{ls} + \varepsilon_{irl}\frac{\partial v_m}{\partial x_k}\frac{\partial Q_{rs}}{\partial x_m}Q_{ls}\right) = \\
\frac{\partial \Omega_i}{\partial x_k} + \frac{1}{2}\varepsilon_{irl}\frac{\partial v_m}{\partial x_k}\frac{\partial Q_{rs}}{\partial x_m}Q_{ls}.
\end{aligned} \tag{5.45}$$

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