

Description of Thermal and Micro-Structural Processes in Generalized Continua: Zhilin's Method and its Modifications

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Abstract The method of description of thermal and micro-structural processes, developed by P.A.Zhilin is discussed. The main idea of the method consists of transformation of the energy balance equation to a special form called the reduced equation of energy balance. This form is obtained by separation of the stress tensors into elastic and dissipative components and introduction of quantities characterizing the physical processes associated with neglected degrees of freedom. As a result the energy balance equation is divided into two or more parts, one of them is the reduced equation of energy balance, and the rest have a sense of heat conduction equation, diffusion equation, equation of structural transformations, etc. We discuss the applicability of this method to generalized continua, in particular, to media with rotational degrees of freedom and media with microstructure. Comparative analysis of various modifications of Zhilin's method, differed in the way of temperature, entropy and chemical potential introduction, is carried out.

1 Introduction

The idea of generalized continua goes back to the work of the Cosserat brothers [6]. The main idea of generalized continua is to consider extra degrees of freedom for material points in order to be able to better model materials with microstructure in the framework of continuum mechanics. Many developments have been reported since

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the seminal work of the Cosserat brothers (see [8, 13, 18, 25, 26] and references therein). One of the most fundamental references on the theory of polar media is the paper written by Kafadar and Eringen [9, 14], where the nonlinear Cosserat medium of a general type is considered. The more recent developments can be seen in [4, 7, 10, 21, 24] and references therein. Due to the effort of Eringen and his contemporaries Cosserat's theory appreciably evolved, however, after a time the interest in studying of the Cosserat 3D-continuum began to wane. One of the reasons was that the attempts to determine the additional elastic moduli experimentally were not successful. At the same time the effect of these constants is so small that in fact the Cosserat theory of elasticity does not provide any improvement in comparison with the classical theory of elasticity.

At the beginning of XXI century a new method of describing of various inelastic processes in solids and multicomponent mixtures by means of the Cosserat continuum was proposed by P. A. Zhilin (see original papers [1, 30–33] and books [34, 35] based on these papers). One of the key ideas of the method consists in the separation of force and moment stresses into elastic and inelastic (dissipative) components. To describe the inelastic processes associated with phase transitions and structural transformations, plastic flow, dynamics of bulk solids, dynamics of granular media, fragmentation and defragmentation of materials, particle diffusion, chemical reactions, etc. it is important to introduce the additional state variables such as temperature, entropy, chemical potential and particle distribution density. In fact, the introduction of these quantities in continuum mechanics should be considered as an attempt to take into account the microstructural processes at the macro level by means of some integral characteristics. Zhilin's method tolerates various modifications of the definitions of entropy and chemical potential as well as other state variables being quantities that cannot be measured. In this paper we consider different ways of introduction of such quantities and carry out their comparative analysis.

The paper is organized as follows. In Sect. 2, in order to describe structure modifications, we introduce the density of particle distribution as an independent characteristic and recall the basic balance equations for the spatial distribution. Following Zhilin [32, 34] in Sect. 3 we rewrite the energy balance equation in a special form called the reduced equation of energy balance. This form is obtained by separation of the stress tensors into elastic and dissipative components and introduction of quantities characterizing the physical processes associated with neglected degrees of freedom. As a result the energy balance equation is divided into two or more parts, one of them is the reduced equation of energy balance, and the rest have a sense of heat conduction equation, equation of structural transformations, etc. Section 4 aims at comparison of Truesdell's and Zhilin's methods of constitutive equations derivation and provides some constitutive equations for the dissipative part of stress tensors. In Sect. 5 we discuss in details the different ways of the entropy and chemical potential introduction and compare these approaches in Sect. 6.

2 Balance Equations for Cosserat Continuum with Microstructure

The majority of the researches were focused on the fact that in a continuum one has to define translations and rotations independently (or in other words, one has to establish force and moment actions as it was done by Euler). Therefore one symmetric stress tensor is not enough to represent the response of the continuum on the external loading. As a result two independent laws of motion appear: the balance of momentum and the balance of angular momentum. Another internal degree of freedom which can be considered explicitly is the distribution of the particle density. Considering this quantity independently of mass density allows to take into account media microstructure changes due to its fragmentation or particle diffusion. Further we formulate the balance equations for a continuum with angular degrees of freedom and microstructure.

Let us choose an inertial reference system and observe the volume V (control volume) fixed in the reference system and containing some amount of body-points. It is assumed that a body-point occupies zero volume and has both translational and angular degrees of freedom. To derive dynamical equations of the continuum we apply the spatial description. Let vector \mathbf{r} determine a position of some point of space. We denote a mass density of the material medium in the point of space by $\rho(\mathbf{r}, t)$, a velocity field by $\mathbf{v}(\mathbf{r}, t)$, fields of rotation tensor and angular velocity vector of the body-point by $\mathbf{Q}(\mathbf{r}, t)$ and $\boldsymbol{\omega}(\mathbf{r}, t)$.

The local form of the mass conservation law can be written as:

$$\frac{\delta \rho}{\delta t} + \rho \nabla \cdot \mathbf{v} = 0. \quad (1)$$

Here $\delta/\delta t$ is the material derivative, ∇ denotes the nabla operator.

In addition to the mass density we introduce a particle density $n(\mathbf{r}, t)$ as an independent variable. Such differentiation is important, for example, when the material tends to fragmentation, as in this case the mass is preserved, but the number of particles changes. In other words considering the particle density as an independent characteristic corresponds to introducing an additional degree of freedom which accounts for structural changes. As a result an additional balance equation for the new variable has to be formulated. This equation can be written by analogy to Eq. (1) with a source term. Thus, the particle balance equations takes the form [1, 35]

$$\frac{\delta n}{\delta t} + n \nabla \cdot \mathbf{v} = \chi. \quad (2)$$

Here χ is the rate of particle production per unit volume.

From combination of Eqs. (1) and (2) it follows that

$$\frac{\delta z}{\delta t} = -\frac{\chi(\mathbf{r}, t)}{n(\mathbf{r}, t)}, \quad z \equiv \ln \left(\frac{\rho(\mathbf{r}, t)n_0(\mathbf{r})}{\rho_0(\mathbf{r})n(\mathbf{r}, t)} \right), \quad (3)$$

where $n_0(\mathbf{r})$ and $\rho_0(\mathbf{r})$ are reference distributions of densities of particles and mass.

To formulate the rest of the balance equations we assume that the kinetic energy of the substance K in the control volume V is an additive function of mass, and thus can be written in terms of a kinetic energy mass density κ

$$K = \int_V \rho \kappa dV.$$

Then, following [32, 35], we postulate that κ is a quadratic form of translational and angular velocities of the body-point

$$\kappa = \frac{1}{2} \mathbf{v} \cdot \mathbf{v} + \mathbf{v} \cdot \mathbf{B} \cdot \boldsymbol{\omega} + \frac{1}{2} \boldsymbol{\omega} \cdot \mathbf{C} \cdot \boldsymbol{\omega}, \quad (4)$$

where $\mathbf{B} = \mathbf{Q} \cdot \mathbf{B}_0 \cdot \mathbf{Q}^T$ and $\mathbf{C} = \mathbf{Q} \cdot \mathbf{C}_0 \cdot \mathbf{Q}^T$ are the mass densities of the inertia tensors of the body-point. \mathbf{B}_0 and \mathbf{C}_0 are the inertia tensors in the reference state per unit mass. \mathbf{Q} is a rotation tensor. It relates to $\boldsymbol{\omega}$ by the equation:

$$\frac{d\mathbf{Q}(\mathbf{r}, t)}{dt} = \boldsymbol{\omega}(\mathbf{r}, t) \times \mathbf{Q}(\mathbf{r}, t)$$

Then the linear momentum is defined by expression

$$\mathbf{K}_1 = \int_V \rho \mathcal{K}_1 dV, \quad \mathcal{K}_1 = \frac{\partial \kappa}{\partial \mathbf{v}} = \mathbf{v} + \mathbf{B} \cdot \boldsymbol{\omega}, \quad (5)$$

where \mathcal{K}_1 is the mass density of momentum.

The angular momentum calculated relative to the origin is defined as:

$$\mathbf{K}_2 = \int_V \rho \mathcal{K}_2 dV, \quad \mathcal{K}_2 = \mathbf{r} \times \mathcal{K}_1 + \mathcal{L}, \quad (6)$$

where

$$\mathcal{L} \equiv \frac{\partial \kappa}{\partial \boldsymbol{\omega}} = \mathbf{v} \cdot \mathbf{B} + \mathbf{C} \cdot \boldsymbol{\omega} \quad (7)$$

is the mass density of the dynamic spin.

Euler's first dynamical law momentum balance equation for the control volume V bounded by smooth surface Σ within the spatial description may be written

$$\frac{d}{dt} \int_V \rho \mathcal{K}_1 dV = \int_V \rho \mathbf{F} dV + \int_{\Sigma} (\mathbf{T}_n - \rho \mathbf{n} \cdot \mathbf{v} \mathcal{K}_1) d\Sigma, \quad (8)$$

where d/dt is the total time derivative, \mathbf{F} is an external force per unit mass, \mathbf{T}_n is a stress vector acting upon an elementary surface, \mathbf{n} is normal to this surface.

The local form of Euler's first dynamical law is:

$$\rho \frac{\delta}{\delta t} \mathcal{K}_1 = \nabla \cdot \mathbf{T} + \rho \mathbf{F}, \quad (9)$$

where \mathbf{T} is the Cauchy stress tensor ($\mathbf{T}_n = \mathbf{n} \cdot \mathbf{T}$).

Euler's second dynamical law (the equation for balance of the angular momentum) within spatial description is as follows:

$$\frac{d}{dt} \int_V \rho \mathcal{K}_2 dV = \int_V \rho (\mathbf{r} \times \mathbf{F} + \mathbf{L}) dV + \int_{\Sigma} (\mathbf{r} \times \mathbf{T}_n + \mathbf{M}_n - \rho \mathbf{n} \cdot \mathbf{v} \mathcal{K}_2) d\Sigma, \quad (10)$$

where \mathbf{L} is an external moment per unit mass, \mathbf{M}_n is a moment acting upon a surface with the normal \mathbf{n} .

Using Euler's first dynamical law one can obtain the local form for Euler's second dynamical law for a generalized continuum

$$\rho \frac{\delta}{\delta t} \mathcal{K}_2 = \nabla \cdot \mathbf{M} + \mathbf{T}_\times + \rho \mathbf{L}, \quad (11)$$

where \mathbf{M} is a couple tensor introduced in analogy to the stress tensor, \mathbf{T}_\times is a vector invariant of a second rank tensor. For the dyad \mathbf{ab} it is defined by $(\mathbf{ab})_\times = \mathbf{a} \times \mathbf{b}$. The material derivative of the angular momentum has the form:

$$\frac{\delta}{\delta t} \mathcal{K}_2 = \mathbf{v} \times \mathcal{K}_1 + \frac{\delta}{\delta t} \mathcal{L} = \mathbf{v} \times \mathbf{B} \cdot \boldsymbol{\omega} + \frac{\delta}{\delta t} \mathcal{L} \quad (12)$$

The first law of thermodynamics (the energy balance equation) states that there is a function of state \mathcal{U} (called internal energy) satisfying the equation

$$\frac{d}{dt} (\mathcal{K} + \mathcal{U}) = N^e + Q, \quad (13)$$

where N^e is the power of external forces, Q is the energy supply from external sources per unit time.

The definition of internal energy is less formal than that of the kinetic energy. As a matter of fact, the internal energy is the energy of motion on degrees of freedom which are ignored in the model under consideration. Indeed, the momentum balance equation and the angular momentum balance equation are obtained by choosing the kinetic energy as a quadratic form of translational and angular velocities corresponding to the translational and rotational degrees of freedom. Other degrees of freedom that are ignored in the kinetic energy are taken into account by means of the internal energy. As a rule the sense of the internal energy depends on the mathematical model

used for description of the system. For example, in classical equilibrium thermodynamics the internal energy of the ideal gas is an additive function of the number of particles and proportional to the temperature [19, 23]. In statistical thermodynamics the internal energy is determined by the elastic interactions of the particles, and for the ideal gas it is equal to zero [16]. The difference between the approaches can not give the cause for doubts about their correctness. The fact is that the internal energy is a quantity that cannot be measured, and so there are no physical experiments which let us know what the internal energy of the system under consideration is.

Usually in many continuum mechanics applications the internal energy is an additive function of the mass [20, 27, 29]. Here we intend to take into account the structure changes in the media caused by a change of the number of particles in the medium. Therefore we suppose that the internal energy is an additive function of the number of particles [32], and we will study the consequences of our supposition. Thus we accept

$$U = \int_V n u \, dV,$$

where u is the specific internal energy.

The power of external forces and coupled forces can be represented in the following form:

$$N^e = \int_V \rho (\mathbf{F} \cdot \mathbf{v} + \mathbf{L} \cdot \boldsymbol{\omega}) \, dV + \int_{\Sigma} (\mathbf{T}_n \cdot \mathbf{v} + \mathbf{M}_n \cdot \boldsymbol{\omega}) \, d\Sigma \quad (14)$$

The energy supply per unit time is determined by the adding (moving away) of new particles to the control volume and by the heat supply per unit time Q which is the sum of the heat supply per unit time directly in the volume V and through the boundary of volume Σ

$$Q = \int_V n q \, dV - \int_{\Sigma} \mathbf{n} \cdot \mathbf{h} \, d\Sigma - \int_{\Sigma} \mathbf{n} \cdot \mathbf{v} (\rho \kappa + n u) \, d\Sigma,$$

where q is the energy supply per unit time into the particles of the medium, \mathbf{h} is the heat flow.

Taking into account Gauss' theorem and balance laws (1), (2), (9) and (11) one can obtain the local form of energy balance equation¹

$$n \frac{\delta u}{\delta t} = n u \frac{\delta z}{\delta t} + \mathbf{T}^T \cdot (\nabla \mathbf{v} + \mathbf{I} \times \boldsymbol{\omega}) + \mathbf{M}^T \cdot \nabla \boldsymbol{\omega} - \nabla \cdot \mathbf{h} + n q, \quad (15)$$

where \mathbf{I} is a unit tensor. However such a form of the energy balance equation is not that good since it is not clear on which arguments the internal energy depends. In

¹ Details are presented in E.N. Vilchevskaya. Appendix: Formula calculus in [35].

the following section we will transform (15) to obtain the so-called reduced energy balance equation.

3 Transformation of the Energy Balance Equation

Let us consider Eq. (15). The right-hand side of this equation contains the power of forces and moments. A part of this power leads to the change of the internal energy. The remaining part of the power is partly conserved within the body as heat and is partly emanated into external medium. In order to separate these parts let us introduce the following decomposition

$$\mathbf{T} = -(p_e + p_f)\mathbf{I} + \boldsymbol{\tau}_e + \boldsymbol{\tau}_f, \quad \mathbf{M} = \mathbf{M}_e + \mathbf{M}_f, \quad \text{tr } \boldsymbol{\tau}_e = \text{tr } \boldsymbol{\tau}_f = 0, \quad (16)$$

where the quantities with the index “e” are independent of velocities. These quantities always affect the internal energy. The quantities with the index “f” account for an internal friction. These quantities may have an influence on the internal energy but only by means of additional parameters like entropy or chemical potential. Taking (16) into account we rewrite the energy balance equation in the form:

$$\begin{aligned} n \frac{\delta u}{\delta t} &= n u \frac{\delta z}{\delta t} - p_e \nabla \cdot \mathbf{v} + \boldsymbol{\tau}_e^T \cdot (\nabla \mathbf{v} + \mathbf{I} \times \boldsymbol{\omega}) + \mathbf{M}_e^T \cdot \nabla \boldsymbol{\omega} \\ &\quad - \nabla \cdot \mathbf{h} + n q - p_f \nabla \cdot \mathbf{v} + \boldsymbol{\tau}_f^T \cdot (\nabla \mathbf{v} + \mathbf{I} \times \boldsymbol{\omega}) + \mathbf{M}_f^T \cdot \nabla \boldsymbol{\omega} \end{aligned} \quad (17)$$

The part of the power of forces and moments that does not depend on velocities can be represented as:

$$\begin{aligned} \boldsymbol{\tau}_e^T \cdot (\nabla \mathbf{v} + \mathbf{I} \times \boldsymbol{\omega}) + \mathbf{M}_e^T \cdot \nabla \boldsymbol{\omega} &= \mathbf{f}_1^T \cdot \frac{\delta \mathbf{E}}{\delta t} + \mathbf{M}_e^T \cdot \frac{\delta \mathbf{F}}{\delta t} + \frac{1}{2} \mathbf{f}_2^T \cdot \frac{\delta \mathbf{Q}}{\delta t} \\ \mathbf{f}_1^T &= -(\boldsymbol{\tau}_e + \mathbf{M}_e \cdot \mathbf{F}^T) \cdot \mathbf{E}^{-T}, \quad \mathbf{f}_2^T = (\mathbf{M}_e^T \cdot \mathbf{F} - \boldsymbol{\tau}_e) \times \mathbf{Q}, \end{aligned} \quad (18)$$

where the strain measure \mathbf{F} and the deformation gradient \mathbf{E} are determined by:

$$\nabla \mathbf{Q} = \mathbf{F} \times \mathbf{Q}, \quad \mathbf{E} = \mathbf{I} - \nabla \mathbf{u} \quad (19)$$

\mathbf{u} is a displacement field. From the mass balance it follows that

$$\nabla \cdot \mathbf{v} = \frac{\rho}{\rho_0} \frac{\delta \sigma}{\delta t}, \quad \sigma = \frac{\rho_0}{\rho} \quad (20)$$

and as a result the energy balance equation takes the form:

$$\begin{aligned}
 n \frac{\delta u}{\delta t} = n u \frac{\delta z}{\delta t} - p_e \frac{\rho}{\rho_0} \frac{\delta \sigma}{\delta t} + \mathbf{f}_1^T \cdot \frac{\delta \mathbf{E}}{\delta t} + \mathbf{M}_e^T \cdot \frac{\delta \mathbf{F}}{\delta t} + \frac{1}{2} \mathbf{f}_2^T \cdot \frac{\delta \mathbf{Q}}{\delta t} \\
 - \nabla \cdot \mathbf{h} + n q - p_f \nabla \cdot \mathbf{v} + \mathbf{\tau}_f^T \cdot (\nabla \mathbf{v} + \mathbf{I} \times \boldsymbol{\omega}) + \mathbf{M}_f^T \cdot \nabla \boldsymbol{\omega}
 \end{aligned} \tag{21}$$

A transformation of the underlined terms is not as formal as the above ones. In order to state the full form of the reduced equation of the energy balance we need to define the concepts of temperature, entropy and chemical potential that will be discussed later.

4 Constitutive Equations

There are several methods of the constitutive equations derivation in continuum mechanics. We start with comparing Zhilin's method with one of the best known and widely used methods—the method of Truesdell.

Truesdell's method [29] is based on the combined use of the first and second laws of thermodynamics. The essence of this method is as follows. The second law of thermodynamics is written in the form of the Clausius–Duhem inequality. Then some thermal terms, namely the rate of heat supply per unit volume and divergence of the heat flow, are excluded from the inequality by means of the energy balance equation. As a result the so-called reduced dissipation inequality is obtained. It must be satisfied for all processes occurring in the medium. Since neither the external mechanical actions nor the heat supply from external sources are included in the reduced dissipation inequality this inequality imposes restrictions to the constitutive equations. In the case of an elastic medium the reduced dissipation inequality allows us to obtain the Cauchy–Green relations for the stress tensor, moment stress tensor and temperature, and imposes restrictions to the choice of the constitutive equation for heat flow vector. After substituting the Cauchy–Green relations into the energy balance equation and performing some mathematical transformations the heat conduction equation is obtained. This equation relates the temperature and entropy, divergence of the heat flow vector and the terms characterizing the rate of heat supply per unit volume. The heat conduction equation closes the system of equations of coupled problem of thermoelasticity. If a medium possesses inelastic properties then the reduced dissipation inequality does not allow us to obtain the constitutive equations in the formal way and only makes it possible to eliminate those constitutive equations which contradict the second law of thermodynamics in the form of the Clausius–Duhem inequality. Thus other methods of the constitutive equations obtaining should be used, for example, the method of rheological models or the method of theory of media with fading memory. At the same time the statement of the heat conduction equation in the form that is obtained in the problem of thermoelasticity is an open question.

The basic idea of Zhilin's method is to transform the energy balance equation into a special form. During this transformation the stresses are represented as a sum of elastic and dissipative components, the temperature and entropy are introduced, and

the energy balance equation is divided into two equations. One of them is the reduced energy balance equation which contains the internal energy, the elastic components of stress tensor and moment stress tensor, and also temperature and entropy. Another equation is the heat conduction equation which contains temperature and entropy, the dissipative components of stress tensor and moment stress tensor, the divergence of the heat flow vector, and the terms characterizing the rate of heat supply per unit volume. In contrast to the reduced dissipation inequality, the reduced energy balance equation used in Zhilin's method allows us to obtain the Cauchy–Green relations for the temperature and the elastic component of the stress tensor in the case of an inelastic medium. Note that by Zhilin's method the Cauchy–Green relations are obtained without use of the second law of thermodynamics, which is used only for the formulation of the constitutive equations for the dissipative components of stress tensors and heat flow vector. In addition, Zhilin's formulation of the second law of thermodynamics differs from the Clausius–Duhem inequality and represents the set of two inequalities [32, 35].

$$\mathbf{h} \cdot \nabla \vartheta \leq 0, \quad \delta = -p_f \nabla \cdot \mathbf{v} + \boldsymbol{\tau}_f^T \cdot (\nabla \mathbf{v} + \mathbf{I} \times \boldsymbol{\omega}) + \mathbf{M}_f^T \cdot \nabla \boldsymbol{\omega} \geq 0, \quad (22)$$

where ϑ is the temperature measured by a thermometer. This formulation is more restrictive than the Clausius–Duhem inequality [28], which follows from Zhilin's formulation.

The first inequality expresses the intuitive condition that heat flows in the direction of the negative gradient of temperature and imposes restriction of the constitutive equation for heat flow vector. The second one can be associated with the statement that the dissipative forces and moments can not perform a positive work and imposes restriction of the constitutive equations for the dissipative components of stress tensors. According to Zhilin [1, 30–35] the components of stress tensors connected with inelastic behavior and internal dissipation can be related with antisymmetric tensors. Below we give some examples of constitutive equations for the dissipative components of stress tensors.

To describe the inelastic behavior of solids, for example, plasticity and dynamics of granular media Zhilin proposed [30–35] the following constitutive equations

$$p_f = 0, \quad \boldsymbol{\tau}_f = \mathbf{I} \times \mathbf{t}, \quad \mathbf{M}_f = \mathbf{0}, \quad (23)$$

where vector \mathbf{t} is determined by analogy with the Coulomb dry friction and takes the form

$$\mathbf{t} = k |\mathbf{n} \cdot \boldsymbol{\tau}_e \cdot \mathbf{n}| \sigma(\mathbf{n} \cdot \boldsymbol{\tau}_e \cdot \mathbf{n}) \frac{2\boldsymbol{\omega} - \nabla \times \mathbf{v}}{|2\boldsymbol{\omega} - \nabla \times \mathbf{v}|}, \quad \boldsymbol{\omega} \neq \frac{1}{2} \nabla \times \mathbf{v}. \quad (24)$$

Here $k > 0$ is the parameter of friction, and the function $\sigma(\mathbf{n} \cdot \boldsymbol{\tau}_e \cdot \mathbf{n})$ is determined as follows

$$\sigma(\mathbf{n} \cdot \boldsymbol{\tau}_e \cdot \mathbf{n}) = \begin{cases} 1, & \mathbf{n} \cdot \boldsymbol{\tau}_e \cdot \mathbf{n} < 0, \\ 0, & \mathbf{n} \cdot \boldsymbol{\tau}_e \cdot \mathbf{n} \geq 0. \end{cases} \quad (25)$$

The unit vector \mathbf{n} in Eq. (24) is found by tensor $\boldsymbol{\tau}_e$ as a solution of the problem

$$\mathbf{n} \cdot \boldsymbol{\tau}_e \cdot \mathbf{m} = \max, \quad \forall \mathbf{n}, \mathbf{m} : |\mathbf{n}| = |\mathbf{m}| = 1, \quad \mathbf{n} \cdot \mathbf{m} = 0. \quad (26)$$

The solution of problem (26) is unique. This fact is proved in [30, 35]. It is easy to see that the constitutive equations (23), (24) satisfy the second law of thermodynamics in the form of Eq. (22). Indeed,

$$\boldsymbol{\tau}_f^T \cdot \cdot (\nabla \mathbf{v} + \mathbf{I} \times \boldsymbol{\omega}) \equiv 2\mathbf{t} \cdot \left(\boldsymbol{\omega} - \frac{1}{2} \nabla \times \mathbf{v} \right). \quad (27)$$

Hence, in view of Eqs. (24), (25) and the fact that $k > 0$ we have

$$\boldsymbol{\tau}_f^T \cdot \cdot (\nabla \mathbf{v} + \mathbf{I} \times \boldsymbol{\omega}) = k |\mathbf{n} \cdot \boldsymbol{\tau}_e \cdot \mathbf{n}| \sigma(\mathbf{n} \cdot \boldsymbol{\tau}_e \cdot \mathbf{n}) |2\boldsymbol{\omega} - \nabla \times \mathbf{v}| \geq 0. \quad (28)$$

All aforesaid relates to the case of sliding. If there is no sliding, i.e. the condition $2\boldsymbol{\omega} = \nabla \times \mathbf{v}$ is satisfied, then vector \mathbf{t} is found from the equations of motion. To be exact, by using the equation of the angular momentum balance vector \mathbf{t} can be excluded from the equation of the momentum balance. Note that if there is no sliding, the friction force is conservative and there is no energy dissipation. In this case the constitutive equations (23) also satisfy the second law of thermodynamics in the form of Eq. (22).

In [32, 35] Zhilin noted that in many cases Coulomb dry friction can be replaced by viscous friction, i.e. instead of Eq. (24) we can use the constitutive equation

$$\mathbf{t} = k \left(\boldsymbol{\omega} - \frac{1}{2} \nabla \times \mathbf{v} \right), \quad (29)$$

where $k > 0$ is the coefficient of viscous friction.

To describe the behavior of a two-component micropolar medium Zhilin proposed [1, 34, 35] the constitutive equations for inelastic components of stress tensors which contain both symmetric and antisymmetric parts. The first component of this medium is a viscous fluid and the second one is a solid-liquid component consisting of fibres.

The constitutive equations for the fluid component are

$$p'_f = 0, \quad \boldsymbol{\tau}'_f = 2\boldsymbol{\mu} \cdot \cdot \mathbf{D} + \mathbf{t}' \times \mathbf{I}, \quad \mathbf{M}'_f = \mathbf{0}, \quad (30)$$

where

$$\mathbf{D} = \frac{1}{2} \left(\nabla \mathbf{v}_1 + \nabla \mathbf{v}_1^T - \frac{2}{3} (\nabla \cdot \mathbf{v}_1) \mathbf{I} \right). \quad (31)$$

Vector \mathbf{t}' is a vector of viscous friction which depends on the particle distribution density of the solid-liquid component:

$$\mathbf{t}' = \eta_2 \mu_1 \cdot \left(\boldsymbol{\omega} - \frac{1}{2} \nabla \times \mathbf{v}_1 \right). \quad (32)$$

The first term in Eq.(30)₂ is a standard term for a viscous fluid. The second term in Eq.(30)₂ characterizes friction due to the presence of a solid-liquid component.

The constitutive equations for the solid-liquid component are

$$p_f'' = 0, \quad \boldsymbol{\tau}_f'' = \mathbf{t}'' \times \mathbf{I}, \quad \mathbf{M}_f'' = \mathbf{m}'' \times \mathbf{I}, \quad (33)$$

where vectors \mathbf{t}'' and \mathbf{m}'' are

$$\mathbf{t}'' = \eta_2 \mu_2 \cdot \left(\boldsymbol{\omega} - \frac{1}{2} \nabla \times \mathbf{v}_2 \right), \quad \mathbf{m} = - \eta_2 \mu_3 (\nabla \times \boldsymbol{\omega}). \quad (34)$$

The tensors of viscous friction coefficients must satisfy the relations

$$\begin{aligned} \forall \mathbf{a}, \mathbf{b}, \mathbf{c} \text{ with } \mathbf{c} = -\mathbf{c}^T : \quad & \mathbf{a} \cdot \boldsymbol{\mu} \cdot \mathbf{a} \geq 0, \quad \mathbf{b} \cdot \boldsymbol{\mu}_1 \cdot \mathbf{b} \geq 0, \quad \mu_3 \geq 0, \\ & \mathbf{a} \cdot \boldsymbol{\mu} = \boldsymbol{\mu} \cdot \mathbf{a}, \quad \mathbf{c} \cdot \boldsymbol{\mu} = \mathbf{0}, \quad \mathbf{I} \cdot \boldsymbol{\mu} = \mathbf{0}, \quad \mathbf{b} \cdot \boldsymbol{\mu}_1 = \boldsymbol{\mu}_1 \cdot \mathbf{b}. \end{aligned} \quad (35)$$

The inelastic components of stress tensors are responsible for the conversion of mechanical energy into heat. In accordance with Zhilin's constitutive equations the transfer of energy into heat is associated with the motion by rotational degrees of freedom, i. e. by those degrees of freedom for which there are no elastic interactions. Note that the classical model of viscous fluid is constructed similarly: the pressure is assumed to be elastic and depends on the mass density (or volume strain, that is the same) whereas the viscous stresses are determined by the deviatoric part of the stress tensor and depend on the deviatoric part of the strain tensor. Thus, in this model of fluid the dissipation of mechanical energy occurs by degrees of freedom without elastic interactions. It is not possible within the framework of classical continuum to implement this principle in relation to the solid where elastic interactions are described by a symmetric stress tensor. The use of a generalized continuum allows us to associate mechanical energy dissipation with the degrees of freedom for which there is no elastic interactions, namely the rotational degrees of freedom which correspond to the moment stress tensor and the antisymmetric parts of the stress tensor.

5 Different Ways of Entropy and Chemical Potential Introduction

Usually the concepts of temperature, entropy, internal energy and chemical potential are supposed to be well-known. However, in fact there are no satisfactory definitions for them in continuum mechanics. The problem is that it is impossible to prove

that the temperature as it is introduced in thermodynamics or in statistical physics coincides with the temperature definition as it is used in continuum mechanics. A situation with the definition of variables that cannot be measured such as the entropy, internal energy or chemical potential is even more complicated. Such quantities are characteristics of a mathematical model and they are necessary for obtaining some relations connecting measurable quantities. Consequently, the preference of this or that definition is determined by specific features of problems under consideration.

In fact, the entropy is introduced as an attempt to take into account a dependence of the internal energy on the velocities of the ignored degrees of freedom. There are different ways of entropy introduction (see [3, 5, 17, 22] for example) and it is difficult to say unambiguously which of them is more preferable. A new thermodynamical quantity—chemical potential is introduced to describe a change of density of particles. As usual in thermodynamics the chemical potential is defined as the derivative of the internal energy with respect to the number of particles [12, 23]. However there exist other definitions of the chemical potential. For example, Baierlein [2] proposed to introduce the chemical potential by describing its properties instead of explaining the chemical potential by relating it to an energy change. These ideas have a further development in [11]. Zhilin [32] suggested a new concept of the chemical potential as a conjugate variable to the number of particles. Its definition is given by means of pure mechanical arguments, which are based on using a special form of the energy balance equation.

Further different ways of the entropy and chemical potential introduction based on the method developed by Zhilin [34, 35] are considered.

5.1 Variant 1

Let us introduce the temperature $\vartheta(\mathbf{r}, t)$ and entropy $\eta(\mathbf{r}, t)$ by the following equation:

$$nq - \nabla \cdot \mathbf{h} - p_f \nabla \cdot \mathbf{v} + \boldsymbol{\tau}_f^T \cdot (\nabla \mathbf{v} + \mathbf{I} \times \boldsymbol{\omega}) + \mathbf{M}_f^T \cdot \nabla \boldsymbol{\omega} = n\vartheta \frac{\delta \eta}{\delta t} \quad (36)$$

The above given definition brings about a few remarks. First, the temperature ϑ is considered to be some characteristic of the medium that is measured by a thermometer, and the entropy η related to one particle is introduced as a quantity conjugate with the temperature. Second, since we suppose that the internal energy is an additive function of the number of particles then it is assumed that the entropy is also an additive function of the number of particles. Note that this definition of entropy is different from the definition used, for example, in classical thermodynamics or physics, where an inequality is introduced. In particular, the proposed definition does not coincide with the concept of an equilibrium process. The Eq. (36) is the heat conduction equation, i.e. equation describing a non-equilibrium process.

Accounting for (36) one may rewrite the Eq. (21) in the form:

$$n \frac{\delta u}{\delta t} = n u \frac{\delta z}{\delta t} - p_e \frac{\rho}{\rho_0} \frac{\delta \sigma}{\delta t} + \mathbf{f}_1^\top \cdot \frac{\delta \mathbf{E}}{\delta t} + \mathbf{M}_e^\top \cdot \frac{\delta \mathbf{F}}{\delta t} + \frac{1}{2} \mathbf{f}_2^\top \cdot \frac{\delta \mathbf{Q}}{\delta t} + n \vartheta \frac{\delta \eta}{\delta t} \quad (37)$$

It is seen that the internal energy is a function of the following arguments

$$u = u(z, \sigma, \eta, \mathbf{E}, \mathbf{F}, \mathbf{Q}) \quad (38)$$

Note that from (38) and (47) it follows that

$$u = \frac{\partial u}{\partial z} \quad (39)$$

In thermodynamics the derivative of the internal energy with respect to the number of particles is usually called chemical potential [12, 23]. Introduction of the temperature and entropy by (36) means that a role of the chemical potential can be played by the internal energy.

Let us show that the variable z can be excluded from the arguments of the internal energy. Indeed from (39) it follows that

$$u = u_*(\sigma, \eta, \mathbf{E}, \mathbf{F}, \mathbf{Q}) \frac{\rho_0}{n_0} \exp z \Rightarrow u = \frac{\rho}{n} u_*, \quad (40)$$

where u_* is a mass density of the internal energy. It should be noted that the last equation is only valid, if there are no massless particles in the system.

Insertion of (39) into (37) gives

$$\begin{aligned} \rho \frac{\delta u_*}{\delta t} = & -\frac{p_e}{\sigma} \frac{\delta \sigma}{\delta t} + n \vartheta \frac{\delta \eta}{\delta t} + (\mathbf{E}^{-1} \cdot \boldsymbol{\tau}_e^\top + \mathbf{E}^{-1} \cdot \mathbf{F} \cdot \mathbf{M}_e^\top) \cdot \frac{\delta \mathbf{E}}{\delta t} \\ & + \mathbf{M}_e^\top \cdot \frac{\delta \mathbf{F}}{\delta t} + \frac{1}{2} ((\mathbf{M}_e^\top \cdot \mathbf{F} - \boldsymbol{\tau}_e) \times \times \mathbf{Q})^\top \cdot \frac{\delta \mathbf{Q}}{\delta t} \end{aligned} \quad (41)$$

From the reduced energy balance equation one can derive the Cauchy-Green relations

$$\begin{aligned} p_e = -\frac{\partial \rho_0 u_*}{\partial \sigma}, \quad \vartheta = \frac{1}{\sigma n} \frac{\partial \rho_0 u_*}{\partial \eta}, \quad \sigma \mathbf{M}_e = \frac{\rho_0 \partial u_*}{\partial \mathbf{F}}, \\ \sigma \boldsymbol{\tau}_e = -\frac{\rho_0 \partial u_*}{\partial \mathbf{E}} \cdot \mathbf{E}^\top - \frac{\rho_0 \partial u_*}{\partial \mathbf{F}} \cdot \mathbf{F}^\top \end{aligned} \quad (42)$$

and constrains which the internal energy has to satisfy

$$\begin{aligned} \left(\frac{\partial u_*}{\partial \mathbf{E}} \right)^\top \cdot \mathbf{E} + \left(\frac{\partial u_*}{\partial \mathbf{F}} \right)^\top \cdot \mathbf{F} = 0, \\ \left(\frac{\partial u_*}{\partial \mathbf{E}} \right)^\top \cdot (\mathbf{A} \cdot \mathbf{E}) + \left(\frac{\partial u_*}{\partial \mathbf{Q}} \right)^\top \cdot (\mathbf{A} \cdot \mathbf{Q}) + \left(\frac{\partial u_*}{\partial \mathbf{F}} \right)^\top \cdot (\mathbf{A} \cdot \mathbf{F} - \mathbf{F} \cdot \mathbf{A}) = 0, \end{aligned} \quad (43)$$

where \mathbf{A} is an arbitrary antisymmetric tensor.

Note that the function $\rho_0 u_*$ is independent of z . It means that only the constitutive equation for the temperature depends on the distribution density of the particles. The heat conduction equation depends on n only by means of $n\vartheta \frac{\delta \eta}{\delta t}$, and the chemical potential does not appear in any equation.

Considering function $\rho_0 u_*$ implies that we assume that the internal energy is an additive function of mass. In this case it is natural to assume that the entropy is also additive by mass. Thus instead of (36) we can introduce the temperature and entropy η_* by means of

$$\rho \mathbf{q}_* - \nabla \cdot \mathbf{h} - p_f \nabla \cdot \mathbf{v} + \boldsymbol{\tau}_f^T \cdot (\nabla \mathbf{v} + \mathbf{I} \times \boldsymbol{\omega}) + \mathbf{M}_f^T \cdot \nabla \boldsymbol{\omega} = \rho \vartheta \frac{\delta \eta_*}{\delta t} \quad (44)$$

Then the reduced equation of the energy balance has the form

$$\begin{aligned} \rho \frac{\delta u_*}{\delta t} = & -\frac{p_e}{\sigma} \frac{\delta \sigma}{\delta t} + \rho \vartheta \frac{\delta \eta_*}{\delta t} + \left(\mathbf{E}^{-1} \cdot \boldsymbol{\tau}_e^T + \mathbf{E}^{-1} \cdot \mathbf{F} \cdot \mathbf{M}_e^T \right) \cdot \frac{\delta \mathbf{E}}{\delta t} \\ & + \mathbf{M}_e^T \cdot \frac{\delta \mathbf{F}}{\delta t} + \frac{1}{2} \left((\mathbf{M}_e^T \cdot \mathbf{F} - \boldsymbol{\tau}_e) \times \times \mathbf{Q} \right)^T \cdot \frac{\delta \mathbf{Q}}{\delta t} \end{aligned} \quad (45)$$

All Cauchy-Green relations (42) are still valid except the one for the temperature, which now has the form

$$\vartheta = \frac{\partial u_*}{\partial \eta_*} \quad (46)$$

It is seen that the heat conduction equation (44) as well as the constitutive equations (42) do not depend on the particle density. Thus the influence of the mechanical and thermal processes on the change of the particle distribution can be taken into account only by means of the source term in the particle balance equation (2). So the stress-strain state and the temperature conditions can affect the changes of particle distribution density since the source term in the particle balance equation can depend on all these factors. Hence, this method of temperature and entropy introduction can be used to describe the structure transformations and phase transitions which occur without the release or absorption of heat and are not accompanied by significant changes in the mechanical and thermodynamical characteristics but only leads to changes in other physical characteristics such as, for example, electrical or magnetic properties.

5.2 Variant 2

An alternative form of the reduced energy balance equation makes use of the particle balance equation. We insert (3) into (21) and obtain

$$n \frac{\delta u}{\delta t} = -p_e \frac{\rho}{\rho_0} \frac{\delta \sigma}{\delta t} + \mathbf{f}_1^T \cdot \frac{\delta \mathbf{E}}{\delta t} + \mathbf{M}_e^T \cdot \frac{\delta \mathbf{F}}{\delta t} + \frac{1}{2} \mathbf{f}_2^T \cdot \frac{\delta \mathbf{Q}}{\delta t} - \chi u - \nabla \cdot \mathbf{h} + nq - p_f \nabla \cdot \mathbf{v} + \boldsymbol{\tau}_f^T \cdot (\nabla \mathbf{v} + \mathbf{I} \times \boldsymbol{\omega}) + \mathbf{M}_f^T \cdot \nabla \boldsymbol{\omega} \quad (47)$$

and as a result the source term in the particle balance equation χ appears in the energy balance equation.

Now let us define the temperature and entropy by the equation

$$-\chi u - \nabla \cdot \mathbf{h} + nq - p_f \nabla \cdot \mathbf{v} + \boldsymbol{\tau}_f^T \cdot (\nabla \mathbf{v} + \mathbf{I} \times \boldsymbol{\omega}) + \mathbf{M}_f^T \cdot \nabla \boldsymbol{\omega} = n\vartheta \frac{\delta \eta}{\delta t} \quad (48)$$

and investigate the consequences. This equation differs from (36) only due to the term χu standing for the energy supply per unit time caused by the structural transitions of the medium. Then the reduced energy balance equation takes the form

$$n \frac{\delta u}{\delta t} = -\frac{p_e}{\sigma} \frac{\delta \sigma}{\delta t} + (\mathbf{E}^{-1} \cdot \boldsymbol{\tau}_e^T + \mathbf{E}^{-1} \cdot \mathbf{F} \cdot \mathbf{M}_e^T) \cdot \frac{\delta \mathbf{E}}{\delta t} + \mathbf{M}_e^T \cdot \frac{\delta \mathbf{F}}{\delta t} + \frac{1}{2} ((\mathbf{M}_e^T \cdot \mathbf{F} - \boldsymbol{\tau}_e) \times \mathbf{Q})^T \cdot \frac{\delta \mathbf{Q}}{\delta t} + n\vartheta \frac{\delta \eta}{\delta t} \quad (49)$$

Thus the internal energy is a function of the following independent arguments

$$u = u(\sigma, \eta, \mathbf{E}, \mathbf{F}, \mathbf{Q}) \quad (50)$$

and the Cauchy-Green relations are

$$p_e = -n\sigma \frac{\partial u}{\partial \sigma}, \quad \vartheta = \frac{\partial u}{\partial \eta}, \quad \sigma \mathbf{M}_e = n \frac{\partial u}{\partial \mathbf{F}}, \quad (51)$$

$$\boldsymbol{\tau}_e = -n \frac{\partial u}{\partial \mathbf{E}} \cdot \mathbf{E}^T - n \frac{\partial u}{\partial \mathbf{F}} \cdot \mathbf{F}^T$$

The constraints for the internal energy u are the same as they were in Variant 1 for u_* .

Note that now the internal energy does not play role of the chemical potential as it was in Variant 1. At the same time the heat conduction equation (48) has a term connected with particle distribution changes and this term depends on the internal energy. Thus, this method of introduction of temperature can be used to describe the structure transformations and phase transitions accompanied by the release or absorption of heat. Note that the first and second variants of derivation of the constitutive equations and the heat conduction equation are correct both in the case when the mass density and the particle distribution density are independent quantities and in the case when they are linearly related (i.e. when the source term in the particle balance equation is equal to zero).

5.3 Variant 3

Let us assume that some part of the underlined terms in (21) is responsible for the change in the number of particles. Therefore, instead of Eq. (36) we will use a more general equation containing an additional term that accounts for structural transitions. We denote

$$nq - \nabla \cdot \mathbf{h} - p_f \nabla \cdot \mathbf{v} + \boldsymbol{\tau}_f^T \cdot (\nabla \mathbf{v} + \mathbf{I} \times \boldsymbol{\omega}) + \mathbf{M}_f^T \cdot \nabla \boldsymbol{\omega} = n\vartheta \frac{\delta \eta}{\delta t} + \psi \frac{\delta n}{\delta t} \quad (52)$$

Analogous to the temperature and entropy, n and ψ appear in Eq. (52) as the conjugate variables. Equation (52) is the combined equation of structural transitions (e.g., fragmentation) and heat conduction.

Substituting Eq. (52) into (21) after some transformation we obtain the reduced energy balance equation in the form

$$\begin{aligned} \frac{\delta(nu)}{\delta t} &= \frac{p_e + nu}{\rho} \frac{\delta \rho}{\delta t} + \mathbf{f}_1^T \cdot \frac{\delta \mathbf{E}}{\delta t} + \mathbf{M}_e^T \cdot \frac{\delta \mathbf{F}}{\delta t} + \frac{1}{2} \mathbf{f}_2^T \cdot \frac{\delta \mathbf{Q}}{\delta t} \\ &+ n\vartheta \frac{\delta \eta}{\delta t} + \psi \frac{\delta n}{\delta t} \end{aligned} \quad (53)$$

It is significant that such a form of the reduced energy balance equation is valid only if the mass density and the density of particle distribution are independent variables.

From Eq. (53) there follow the Cauchy-Green relations

$$\begin{aligned} p_e &= \rho^2 \frac{\partial}{\partial \rho} \left(\frac{nu}{\rho} \right), & \vartheta &= \frac{1}{n} \frac{\partial(nu)}{\partial \eta}, & \psi &= \frac{\partial(nu)}{\partial n}, \\ \mathbf{M}_e &= \frac{\partial(nu)}{\partial \mathbf{F}}, & \boldsymbol{\tau}_e &= - \frac{\partial(nu)}{\partial \mathbf{E}} \cdot \mathbf{E}^T - \frac{\partial(nu)}{\partial \mathbf{F}} \cdot \mathbf{F}^T \end{aligned} \quad (54)$$

From Eq. (54)₃ it is seen that ψ is a chemical potential. Similar expressions to (54)₃ are given in the classical textbooks [15, 19, 20, 23].

Note that Eq. (52) characterizes only overall influence of the entropy and chemical potential on the internal energy. To clarify their roles in the considered processes it is necessary to split Eq. (52) into two equations: the heat conduction equation and the equation of structural transitions.

$$n\vartheta \frac{\delta \eta}{\delta t} + Q = nq_1 - \nabla \cdot \mathbf{h}_1 - p_1 \nabla \cdot \mathbf{v} + \boldsymbol{\tau}_f^T \cdot (\nabla \mathbf{v} + \mathbf{I} \times \boldsymbol{\omega}) + \mathbf{M}_f^T \cdot \nabla \boldsymbol{\omega}, \quad (55)$$

$$\psi \frac{\delta n}{\delta t} - Q = nq_2 - \nabla \cdot \mathbf{h}_2 - p_2 \nabla \cdot \mathbf{v} \quad (56)$$

Where the following decompositions are used

$$\mathbf{h} = \mathbf{h}_1 + \mathbf{h}_2, \quad \mathbf{q} = \mathbf{q}_1 + \mathbf{q}_2, \quad p_f = p_1 + p_2 \quad (57)$$

The equivalence of Eqs. (52) and (55) is determined by the presence of the undefined quantity Q characterizing the rate of energy exchange in the processes of the heat conductivity and the structural transitions.

The definition (55) given above brings about a necessity to formulate constitutive equations for all new quantities: \mathbf{h}_i , \mathbf{q}_i , p_i ($i = 1, 2$) and Q . The following circumstances have to be taken into account. First, suppose that the expression for the internal energy u and the source term χ are given. Then we have two equations for n and ψ —the particle balance equation, and Cauchy-Green relation relating these quantities. It means that the term $\psi \frac{\delta n}{\delta t}$ in the equation of structural transformations is determined. Therefore the constitutive equations for \mathbf{h}_2 , \mathbf{q}_2 , p_2 and Q can not be independent. Second, arbitrarily given constitutive equations for \mathbf{h}_2 , \mathbf{q}_2 , p_2 and Q together with the equation of structural transitions and corresponding Cauchy-Green relation determines the quantities n and ψ . Then the particle balance equation allows us to determine the source term χ . Finally a third variant exists. We can arbitrarily choose the constitutive equations for \mathbf{h}_2 , \mathbf{q}_2 , p_2 , Q and χ , but in this case there is no freedom in choosing internal energy.

Introduction of the chemical potential as an independent variable is necessary to describe the diffusion processes and chemical reactions as well as the structure transformations and phase transitions which are accompanied by the release or absorption of heat and occur at a constant temperature.

6 Discussion

The investigation carried out shows that the mass density and particle density can be considered as independent variables without the chemical potential introduction. In some cases the role of the chemical potential can be played by the internal energy or the source term in the particle balance equation. Of course there is no reason to say that there is no necessity for the chemical potential introduction in general. The preference of this or that approach is determined by specific features of the problems under consideration. For example, if experimental data allow us to formulate the constitutive equation for the quantity Q characterizing the rate of energy exchange in the processes of the heat conductivity and the structural transitions, then the third variant of unmeasurable parameters introduction looks more preferable. In the opposite case an approach based on smaller amount of the constitutive equations should be chosen. The first and the second approaches require only the source term χ specification and do not impose any constraints on the internal energy definition. Thus they are easier in this sense, but of course a number of problems stays beyond the consideration.

Also it is important to lay stress on the fact that the equations of structural transitions and heat conduction (44), (48) and (52) define not only the entropy and chemical

potential but also the internal energy. Thus all these quantities should be introduced simultaneously.

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