

## THERMODYNAMIC METHOD FOR CONSTRUCTING CONSTITUTIVE RELATIONS FOR MODELS OF CONTINUOUS MEDIA

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A thermodynamic method is considered for formulation of constitutive relations for models of continuous media. The method is based on the inequality for free energy and on the concept of the parameters of state. We suggest a modification of this method that does not require involving additional principles for the dissipation rate and applies to a broader class of constitutive relations. The utilization of this method is demonstrated by a number of cases of the formulation of constitutive relations for familiar models of gaseous, liquid, and solid media.

1. The construction of new constitutive relations has been basically motivated by the desire to reproduce theoretically the results of physical experiments that fail to be described with an acceptable accuracy by available constitutive relations. The new relations must agree with the available ones in the regions where the latter relations demonstrate reasonably high accuracy. Also, the new relations must be well-defined in terms of physics and mathematics. This means that these relations must satisfy the principles of thermodynamics, dimensional analysis, invariance, and objectivity.

An approach to the construction of constitutive relations which can be clearly interpreted in terms of physics and mathematics is based on the concept of the parameters of state and the inequality for free energy [1–14]. Since the number of publications developing this approach is extremely large and it is impossible to cite all of them, we cite only those of the publications on which the method suggested has been directly based. In the cited works, one can find additional references.

Although the approach in question has been developed in numerous investigations since the 1950th and can be regarded traditional, its systematic presentation has been absent from the literature. For that reason, we chose to give the basic principles of this approach in the present paper. The scheme suggested for thermodynamic formulation of constitutive relations has been worked out after the analysis of a great number of publications to realize the general features inherent in this approach and to get rid of some inconsistencies and gaps. In our opinion, systematic utilization of this approach would be helpful for profound understanding of physical and mathematical foundations of constitutive relations, both available and new ones.

Thermodynamic analysis shows that rheological properties of a continuous medium are defined by a set of intrinsic parameters of state of an infinitesimal volume of the medium and the dependence of the free energy and the dissipation rate on these parameters. The constitutive relations for entropy, stresses, and heat fluxes, as well as the kinetic equations for the structural parameters of state follow from these dependences.

To exemplify this approach, we will consider a unified formulation of known relations for an ideal and viscous heat conducting gas, as well as for elastic, elastoplastic, and elastoviscoplastic media. In addition, we will construct relations governing damage processes in elastoviscoplastic media and geomaterials.

2. We will briefly outline some definitions and relations between material and spatial tensors characterizing the state of an infinitesimal volume of a continuum. The spatial tensors—the strain tensor  $\epsilon$  (Almansi tensor) and the strain rate tensor  $\mathbf{e}$  (Euler tensor)—are defined by

$$d\mathbf{x} = \mathbf{F} \cdot d\dot{\mathbf{x}}, \quad d\mathbf{x}^T \cdot d\mathbf{x} - d\dot{\mathbf{x}}^T \cdot d\dot{\mathbf{x}} = d\mathbf{x}^T \cdot 2\epsilon \cdot d\mathbf{x}, \quad \frac{d}{dt}(d\mathbf{x}) = \mathbf{L} \cdot d\mathbf{x}, \quad \frac{d}{dt}(d\mathbf{x}^T \cdot d\mathbf{x}) = d\mathbf{x}^T \cdot 2\mathbf{e} \cdot d\mathbf{x}, \quad (2.1)$$

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where  $\mathbf{F}$  and  $\mathbf{L}$  are the strain gradient and velocity gradient tensors, respectively. The circle atop a symbol indicates that this symbol is related to the reference (initial) configuration. The law of motion reads  $\mathbf{x} = \mathbf{x}(\mathring{\mathbf{x}}, t)$ . Equations (2.1) imply the following relations between  $\mathbf{F}$ ,  $\epsilon$ ,  $\mathbf{L}$ , and  $\mathbf{e}$ :

$$\mathbf{L} = \frac{d\mathbf{F}}{dt} \cdot \mathbf{F}^{-1}, \quad \epsilon = \frac{1}{2}(\mathbf{I} - \mathbf{F}^{-T} \cdot \mathbf{F}^{-1}), \quad \mathbf{e} = \frac{1}{2}(\mathbf{L} + \mathbf{L}^T), \quad \mathbf{e} = \frac{d\epsilon}{dt} + \epsilon \cdot \mathbf{L} + \mathbf{L}^T \cdot \epsilon, \quad (2.2)$$

where  $\mathbf{I}$  is the identity tensor.

The density  $\rho$ , the spatial stress tensor (Cauchy tensor)  $\sigma$ , and the spatial vector of diffusion heat flux  $\mathbf{q}$  are defined as

$$dm = \rho dV, \quad d\mathbf{P} = \sigma \cdot \mathbf{n} dS, \quad dQ = \mathbf{q} \cdot \mathbf{n} dS, \quad (2.3)$$

where  $dm$  is the mass of an infinitesimal volume  $dV$  in the updated configuration,  $d\mathbf{P}$  is the force acting on an infinitesimal area  $dS$  with the unit normal  $\mathbf{n}$ , and  $dQ$  is the quantity of heat diffused through the area  $dS$  per unit time. The density satisfies the law of conservation of mass (the continuity equation)

$$\frac{d\rho}{dt} + \rho \mathbf{e} : \mathbf{I} = 0, \quad \text{or} \quad \frac{\rho}{\rho_0} = \det(\mathbf{F}^{-1}), \quad (2.4)$$

where  $\rho_0$  is the initial density.

The material tensors of strains,  $\mathring{\epsilon}$ , strain rates,  $\mathring{\mathbf{e}}$ , and stresses,  $\mathring{\sigma}$  are defined by

$$d\mathbf{x}^T \cdot d\mathbf{x} - d\mathring{\mathbf{x}}^T \cdot d\mathring{\mathbf{x}} = d\mathring{\mathbf{x}}^T \cdot \mathring{\epsilon} \cdot d\mathring{\mathbf{x}}, \quad \frac{d}{dt}(d\mathbf{x}^T \cdot d\mathbf{x}) = d\mathring{\mathbf{x}}^T \cdot 2\mathring{\mathbf{e}} \cdot d\mathring{\mathbf{x}}, \quad \mathring{\sigma} : \mathring{\mathbf{e}} = \sigma : \mathbf{e}$$

and are related to the spatial measures by

$$\mathring{\epsilon} = \mathbf{F}^T \cdot \epsilon \cdot \mathbf{F}, \quad \mathring{\mathbf{e}} = \mathbf{F}^T \cdot \mathbf{e} \cdot \mathbf{F}, \quad \mathring{\sigma} = \mathbf{F}^{-1} \cdot \sigma \cdot \mathbf{F}^{-T}, \quad \frac{d\mathring{\epsilon}}{dt} = \mathring{\mathbf{e}}. \quad (2.5)$$

**3.** Let us consider the thermodynamic foundations of the method suggested. The general laws of thermodynamics for non-equilibrium irreversible thermomechanical processes read

$$\rho \frac{dU}{dt} = \sigma : \mathbf{e} + \rho r + \nabla \cdot \mathbf{q}, \quad \rho \frac{d\eta}{dt} - \nabla \cdot \left( \frac{\mathbf{q}}{T} \right) - \frac{\rho r}{T} \geq 0,$$

where the internal energy  $U$ , the internal heat sources  $r$ , and the entropy  $\eta$  are measured per unit mass;  $T$  is temperature,  $\sigma$  is the Cauchy stress tensor,  $\mathbf{e}$  is the Euler strain rate tensor, and  $\mathbf{q}$  is the heat flux. The first equation expresses the law of conservation of energy, and the second equation the law of entropy growth. The thermodynamic laws imply the inequality for free energy  $\varphi = U - T\eta$ :

$$-\rho \frac{d\varphi}{dt} - \rho \eta \frac{dT}{dt} + \sigma : \mathbf{e} + \mathbf{q} \cdot \frac{\nabla T}{T} \geq 0. \quad (3.1)$$

This inequality does not involve external variables (such as those characterizing heat sources) and is valid for any thermomechanical process defined by a set of parameters of state.

When deriving the constitutive relations we will use the material tensors along with the spatial tensors. This simplifies the calculations, since the rates of the material tensors are defined by conventional material derivatives with respect to time, whereas for the spatial tensors this would have required taking into account the rotation and deformation of an infinitesimal volume of the continuum (see Eqs. (2.2) and (2.5)). The latter would have caused unnecessary complications.

The set of the parameters of state depends on the class of continuous media to be considered. In general, the number of parameters of state can be infinite, as is the case, for example, for viscoelastic media of integral type. (The thermodynamics of such media has been considered in detail in [6].) To make the presentation clearer, we expound a scheme suggested for thermodynamic formulation of constitutive relations for a simpler case where the number of the parameters of state is finite.

Consider the following set of independent parameters of state:

$$\pi = \left( T, \mathring{\epsilon}, \mathring{\chi}, \frac{dT}{dt}, \mathring{\mathbf{e}}, \frac{d\mathring{\chi}}{dt}, \nabla T \right), \quad (3.2)$$

where  $\dot{\chi}$  are the parameters of state responsible for the processes of change of the internal structure, such as plastic flow, fracture, or sintering. These parameters do not occur explicitly in the inequality for free energy and are introduced to take into account the influence of the loading history. These parameters are defined by differential (with respect to time) equations (kinetic equations) which will be considered in what follows. Continuous media whose behavior is governed by the kinetic equations are referred to as differential media.

In what follows, we assume that the set of parameters  $\pi$  contains a minimum of components and is complete. This means that the rates of change of the parameters of (3.2) are mutually independent and that all other parameters (e.g., entropy, stresses, and heat fluxes) are functions of the components of  $\pi$ . In particular, this is the case for free energy, i.e., we have

$$\varphi = \varphi(\pi).$$

With reference to (3.2) and the last relation, one can rewrite inequality (3.1) as follows:

$$\begin{aligned} -\rho \left( \eta + \frac{\partial \varphi}{\partial T} \right) T_t + \left( \dot{\sigma} - \rho \frac{\partial \varphi}{\partial \dot{\epsilon}} \right) : \dot{\epsilon} - \rho \frac{\partial \varphi}{\partial \dot{\chi}} : \frac{d\dot{\chi}}{dt} + \mathbf{q} \cdot \frac{\nabla T}{T} \\ - \rho \frac{\partial \varphi}{\partial T_t} : \frac{dT_t}{dt} - \rho \frac{\partial \varphi}{\partial \dot{\epsilon}} : \frac{d\dot{\epsilon}}{dt} - \rho \frac{\partial \varphi}{\partial \dot{\chi}_t} : \frac{d\dot{\chi}_t}{dt} - \rho \frac{\partial \varphi}{\partial \nabla T} : \frac{d\nabla T}{dt} \geq 0. \end{aligned} \quad (3.3)$$

The derivatives  $dT_t/dt$ ,  $d\dot{\epsilon}/dt$ ,  $d\dot{\chi}/dt$ , and  $d\nabla T/dt$  do not belong to the set of the parameters of state (3.2), whereas the coefficients of these derivatives are functions of the parameter of (3.2). Therefore, the occurrence of the terms with these derivatives violates inequality (3.3) and the laws of thermodynamics, and it is necessary that

$$\frac{\partial \varphi}{\partial T_t} = 0, \quad \frac{\partial \varphi}{\partial \dot{\epsilon}} = 0, \quad \frac{\partial \varphi}{\partial \dot{\chi}_t} = 0, \quad \frac{\partial \varphi}{\partial \nabla T} = 0.$$

Hence, the free energy depends on part of the parameters of state, namely,

$$\varphi = \varphi(\pi^{(1)}), \quad \pi^{(1)} = (T, \dot{\epsilon}, \dot{\chi}).$$

Then inequality (3.1) takes the form of the dissipation inequality

$$-\rho \left( \eta + \frac{\partial \varphi}{\partial T} \right) \frac{dT}{dt} + \left( \dot{\sigma} - \rho \frac{\partial \varphi}{\partial \dot{\epsilon}} \right) : \dot{\epsilon} - \rho \left( \frac{\partial \varphi}{\partial \dot{\chi}} \right) : \frac{d\dot{\chi}}{dt} + \mathbf{q} \cdot \frac{\nabla T}{T} \geq 0, \quad (3.4)$$

where the four groups of terms represent the basic dissipation processes: irreversible growth of entropy, diffusion of the momentum, structural changes in the continuum, and heat diffusion.

The general solution of the dissipation inequality yields the desired constitutive relations

$$\begin{aligned} -\rho \left( \eta + \frac{\partial \varphi}{\partial T} \right) &= -\rho \eta_D \left( T, \dot{\epsilon}, \dot{\chi}, \left[ \frac{dT}{dt} \right], \dot{\epsilon}, \frac{d\dot{\chi}}{dt}, \nabla T \right), \\ \dot{\sigma} - \rho \frac{\partial \varphi}{\partial \dot{\epsilon}} &= \dot{\sigma}_D \left( T, \dot{\epsilon}, \dot{\chi}, \frac{dT}{dt}, [\dot{\epsilon}], \frac{d\dot{\chi}}{dt}, \nabla T \right), \\ -\rho \frac{\partial \varphi}{\partial \dot{\chi}} &= \rho \dot{\chi}_D \left( T, \dot{\epsilon}, \dot{\chi}, \frac{dT}{dt}, \dot{\epsilon}, \left[ \frac{d\dot{\chi}}{dt} \right], \nabla T \right), \\ \frac{\mathbf{q}}{T} &= \frac{1}{T} \mathbf{q}_D \left( T, \dot{\epsilon}, \dot{\chi}, \frac{dT}{dt}, \dot{\epsilon}, \frac{d\dot{\chi}}{dt}, [\nabla T] \right), \end{aligned} \quad (3.5)$$

where square brackets enclosing some arguments do not stand for any mathematical operations and will be explained below. The functions  $Z_1 = -\rho \eta_D$ ,  $Z_2 = \dot{\sigma}_D$ ,  $Z_3 = \rho \dot{\chi}_D$ , and  $Z_4 = \mathbf{q}_D/T$  are referred to as dissipative fluxes or dissipative forces. These functions must satisfy the dissipation rate inequality which takes the form

$$D = -\rho \eta_D(\dots) \frac{dT}{dt} + \dot{\sigma}_D(\dots) : \dot{\epsilon} + \rho \dot{\chi}_D(\dots) : \frac{d\dot{\chi}}{dt} + \frac{1}{T} \mathbf{q}_D(\dots) \cdot \nabla T \geq 0. \quad (3.6)$$

In the particular case of reversible processes, the functions  $\eta_D(\pi)$ ,  $\dot{\sigma}_D(\pi)$ ,  $\mathbf{q}_D(\pi)$ , and  $\dot{\chi}_D(\pi)$  vanish, and inequality (3.6) becomes an equality. So, to formulate the constitutive relations it is necessary to specify the set of parameters of

state and construct two functions—the free energy function,  $\varphi$ , and the dissipation rate function,  $D$ . When constructing these functions, one should be governed by physical considerations concerning the properties of the medium.

The dissipative fluxes or forces  $Z_i$  ( $-\rho\eta_{\text{D}}$ ,  $\dot{\sigma}_{\text{D}}$ ,  $\rho\dot{\chi}$ , and  $\mathbf{q}_{\text{D}}/T$ ) should be constructed together with the dissipation rate function to satisfy the dissipation rate inequality. This completes the problem of construction of the constitutive relations. To satisfy the principles of invariance and objectivity, it suffices to provide that the form of the free energy and dissipation rate functions is invariant to orthogonal transformations of the initial and updated (actual) configurations and to the choice of an inertial reference frame. To meet these requirements it is sufficient for the functions  $\varphi(\pi^{(1)})$  and  $D(\pi^{(1)}, \pi^{(2)})$  to depend only on the tensor invariants of the parameters of state satisfying these conditions.

One can also seek the solution of the dissipation rate inequality among narrower classes of functions describing the basic dissipative processes. For example, one can require each component of the dissipation rate,  $D_i = Z_i \pi_i^{(2)}$ , to be a homogeneous function corresponding to the generalized velocity  $\pi_i^{(2)}$ , where

$$\pi^{(2)} = \left( \frac{dT}{dt}, \dot{\mathbf{e}}, \frac{d\dot{\chi}}{dt}, \nabla T \right), \quad Z = \left( -\rho\eta_{\text{D}}, \dot{\sigma}_{\text{D}}, \rho\dot{\chi}_{\text{D}}, \frac{q_{\text{D}}}{T} \right).$$

(In the general constitutive relations (3.5), the arguments in which the corresponding function is homogeneous are enclosed in square brackets.) In this case, in accordance with Euler's homogeneous function theorem, the expressions for dissipative fluxes take the form

$$Z_i = k_i \frac{\partial D_i}{\partial \pi_i^{(2)}}, \quad k_i = \frac{D_i}{(\partial D_i / \partial \pi_i^{(2)}) : \pi_i^{(2)}}, \quad (3.7)$$

where  $k_i^{-1}$  is the degree of homogeneity of the function  $D_i$ . This is the particular class of solutions that is defined by Ziegler's extremum principle [9] or Onsager's theory [3].

The general constitutive relations of (3.5) leave more room for constructing models of continuous media and give wider possibilities for justifying empirical models or/and those based on the principles of micromechanics and physics of continuum.

**4.** We will demonstrate on familiar models of continuous media how one can derive constitutive relations by using the scheme outlined above. To obtain the constitutive relations one should (i) indicate the processes that are essential for the medium in question and introduce appropriate parameters of state (3.2); (ii) construct expressions for the free energy and the dissipation rate; and (iii) make use of relations (3.5).

The procedure of constructing constitutive relations to a great extent resembles a game, in the sense that one must get what one has laid. The scheme described above establishes rules for such a game which constrain a flight of fancy and ensure a result corresponding to the basic laws and principles of thermomechanics.

Prior to considering examples, we will make a number of important remarks. Note that the density is not an independent parameter of state, since the rate of its change is determined by one of the basic parameters of state, the strain rate tensor, in accordance with the continuity equation (2.4). We especially note the necessity to pass to the material measures of the tensor variables when performing calculations. This passion is not burdensome but simplifies calculations thereby preventing possible errors. After deriving the constitutive relations, one can return spatial tensors. Spatial tensors frequently turn out to be more convenient for solving problems (for example, problems of aeromechanics, aeroelasticity, high-speed impact of solids, or explosion). The abstract tensor notation (see, e.g., [13]) adopted here is also more convenient for mathematical manipulations with the constitutive relations. It permits one to avoid mismatches which may happen when operating with the components of tensors referred to systems of basis vectors corresponding to different configurations. The apparent form of the relations in terms of tensor components may look similar to that of the abstract tensor relations, however, depending on the vector basis, these two forms of relations may express quite different laws. For this reason, to compare constitutive relations, one should consistently use the same forms for representing tensor relations.

**4.1.** Consider the Navier–Stokes model of viscous heat conducting medium. It can be defined as a medium which (i) accumulates heat (the free energy depends on temperature), (ii) resists the volumetric compression (the free energy depends on the density), (iii) does not remember the initial state (is independent on the initial density), and (iv) provides diffusion property for the momentum and heat (the dissipation rate depends on the strain rate and the temperature gradient). In the first approximation, these properties can be formulated as

$$\varphi = \varphi_1(T, \rho), \quad D = \lambda_{\text{V}}(\mathbf{e} : \mathbf{I})^2 + 2\mu_{\text{V}}\mathbf{e} : \mathbf{e} + \frac{k_{\text{q}}}{T}\nabla T \cdot \nabla T,$$

where  $\mathbf{I}$  is the identity tensor,  $\lambda_V$  and  $\mu_V$  are viscosity coefficients, and  $k_q$  is the heat conductivity factor. Note that we use invariants of spatial strain rate tensors to represent the dissipation rate. In terms of the material tensors, the expression for the dissipation rate becomes

$$D = (\lambda_V(\mathbf{F}^{-1} \cdot \mathbf{F}^{-T} : \dot{\mathbf{e}}) \mathbf{F}^{-1} \cdot \mathbf{F}^{-T} + 2\mu_V \mathbf{F}^{-1} \cdot \mathbf{F}^{-T} \cdot \dot{\mathbf{e}} \cdot \mathbf{F}^{-1} \cdot \mathbf{F}^{-T}) : \dot{\mathbf{e}} + \frac{k_q}{T} \nabla T \cdot \nabla T.$$

In what follows, we also proceed to material tensors in a similar way. However, after appropriate calculations, we return to spatial tensors to represent the final result. We will omit the intermediate manipulations.

The constitutive relations for a compressible viscous gas have the usual form independent of the initial configuration of the continuum

$$\eta = \eta_C = -\frac{\partial \varphi_1}{\partial T}, \quad \boldsymbol{\sigma} = \boldsymbol{\sigma}_C + \boldsymbol{\sigma}_D, \quad \boldsymbol{\sigma}_C = -p\mathbf{I}, \quad p = \rho^2 \frac{\partial \varphi}{\partial \rho}, \quad \boldsymbol{\sigma}_D = \lambda_V(\mathbf{e} : \mathbf{I})\mathbf{I} + 2\mu_V \mathbf{e}, \quad \mathbf{q} = k_q \nabla T, \quad U = U_C = \varphi_1 - T \frac{\partial \varphi_1}{\partial T}.$$

The subscript C identifies conservative components depending on the free energy, while the subscript D identifies dissipative components depending on the dissipation rate. For the particular case of an ideal gas, the free energy is expressed as

$$\varphi_1(T, \rho) = C_V T \left( (\gamma - 1) \ln \frac{\rho}{\rho_1} - \ln \frac{T}{T_1} \right)$$

where  $C_V$  is the heat capacity at constant volume,  $\gamma$  is the ratio of heat capacity at constant pressure to that at constant volume, and  $\rho_1$  and  $T_1$  are arbitrary fixed values of the density and temperature, respectively. The relations for entropy, pressure and internal energy are given by

$$\eta = \eta_C = C_V \left( 1 - (\gamma - 1) \ln \frac{\rho}{\rho_1} + \ln \frac{T}{T_1} \right), \quad p = (\gamma - 1)\rho U, \quad U = C_V T.$$

In the particular case of an incompressible medium, the free energy is independent of the density and the pressure is determined by the incompressibility condition.

4.2. Consider a nonlinear thermoelastic isotropic heat conducting medium. It can be defined as a medium which accumulates heat and remembers the initial undeformed state (the free energy depends on temperature and strain; the minimum of the free energy with respect to strains corresponds to the undeformed state in which all strains are zero). For a thermoelastic medium with large volumetric strains and small shear strains, the free energy and the dissipation rate can be expressed, in the first approximation, as

$$\begin{aligned} \varphi &= \varphi_1(T, \rho) + h_1 \frac{\mu(T, \rho)}{\rho} \boldsymbol{\epsilon}' : \boldsymbol{\epsilon}', \\ D_1 &= D_2 = D_3 = 0, \quad D = D_4 = \frac{k_q}{T} \nabla T \cdot \nabla T, \end{aligned}$$

where  $\mu = \mu(T, \rho)$  is the shear modulus and  $h_1 = [1 - \frac{2}{3}(\boldsymbol{\epsilon} : \mathbf{I})]^{-1}$ . The constitutive relations have the form

$$\begin{aligned} \eta = \eta_C &= -\frac{\partial \varphi_1}{\partial T} - h_1(\boldsymbol{\epsilon}' : \boldsymbol{\epsilon}') \frac{1}{\rho} \frac{\partial \mu}{\partial T}, \quad \boldsymbol{\sigma} = \boldsymbol{\sigma}_C = -p\mathbf{I} + 2\mu \boldsymbol{\epsilon}', \quad p = \rho^2 \frac{\partial \varphi_1}{\partial \rho}, \quad \mathbf{q} = k_q \nabla T, \\ U = U_C &= \varphi - T \frac{\partial \varphi}{\partial T} = \varphi_1(T, \rho) + \frac{h_1 \mu}{\rho} (\boldsymbol{\epsilon}' : \boldsymbol{\epsilon}') - T \left( \frac{\partial \varphi_1}{\partial T} + \frac{h_1}{\rho} \frac{\partial \mu}{\partial T} (\boldsymbol{\epsilon}' : \boldsymbol{\epsilon}') \right). \end{aligned}$$

In the particular case where

$$\varphi_1(T, \rho) = \frac{K}{2\rho_0} \left( \ln \frac{\rho}{\rho_0} \right)^2 - K\beta T \ln \frac{\rho}{\rho_0}$$

the pressure is expressed by the simple relation

$$p = K \frac{\rho}{\rho_0} \left( \ln \frac{\rho}{\rho_0} - \beta T \right),$$

where  $K$  is the bulk modulus and  $\beta$  is the temperature coefficient of thermal expansion.

4.3. We proceed now to the analysis of media with structural parameters of state. Consider first a thermoelastoviscoplastic medium. Like an elastic medium, it accumulates heat (the free energy depends on temperature) and the strain energy (the free energy depends on the strain), but its unloaded state (defined as a minimum of the free energy with respect to the strain) corresponds to a nonzero strain  $\epsilon = \epsilon_p$  referred to as the plastic strain. The plastic strain tensor  $\epsilon_p$  characterizes the structural changes in a continuous medium due to the nucleation, growth, and motion of dislocations. This tensor is one of the internal structural parameters  $\chi$ ; it is not associated with any displacement field and does not satisfy the compatibility relations for strains. Therefore, the concept of kinematics does not make sense for plastic strains. The concept of “unloaded configuration” makes sense only in the local interpretation, i.e., as applied to a neighborhood of a particle [15]. The plastic strain tensor is governed by a special kinetic equation referred to as the plastic flow rule. The thermodynamic derivation of this equation will be given below.

For an elastoviscoplastic medium, the free energy is a function of temperature, strain, and plastic strain. The plastic strain tensor identifies a point in the strain space at which the free energy attains a minimum with respect to the strain. The dissipation rate depends on the plastic strain rate (irreversible changes in the structure of the medium) and the temperature gradient (dissipation of heat).

The material tensor of plastic strain rate is defined as the material time derivative of the plastic strain tensor,  $\dot{\epsilon}_p = d\epsilon_p/dt$ . It is convenient to define the corresponding spatial tensors by analogy with the usual strain and strain rate tensors as follows (see (2.5)):

$$\epsilon_p = \mathbf{F}^{-T} \cdot \dot{\epsilon}_p \cdot \mathbf{F}^{-1}, \quad \mathbf{e}_p = \mathbf{F}^{-T} \cdot \dot{\mathbf{e}}_p \cdot \mathbf{F}^{-1}, \quad \mathbf{e}_p = \frac{d\epsilon_p}{dt} + \epsilon_p \cdot \mathbf{L} + \mathbf{L}^T \cdot \epsilon_p.$$

The tensor  $\epsilon - \epsilon_p$  characterizes the deflection of the strain state of the medium from the unloaded state and is referred to as the elastic strain tensor. For plastically incompressible media with large volumetric elastic strains and small shear elastic strains, one can express the free energy and the dissipation rate as follows:

$$\varphi = \varphi_1(T, \rho) + h_1 \frac{\mu}{\rho} [(\epsilon' - \epsilon'_p) : (\epsilon' - \epsilon'_p)], \quad D = H \left( \boldsymbol{\sigma}' : \boldsymbol{\sigma}' - \frac{k_p^2 f_p^2}{\mathbf{e}'_p : \mathbf{e}'_p} \right) k_p f_p (\mathbf{e}'_p : \mathbf{e}'_p) + \frac{k_p}{T} \nabla T \cdot \nabla T,$$

where the plastic strain is represented by the deviatoric tensor  $\epsilon'_p = \frac{1}{3}(\epsilon_p : \mathbf{I}) \mathbf{I}$ ,  $k_q = k_q(T, \rho, \epsilon'_p : \epsilon'_p)$  and  $k_p = k_p(T, \rho, \epsilon'_p : \epsilon'_p)$  are functions of temperature and strains,  $H(\xi)$  is the Heaviside unit step function equal to zero for negative values of the argument and unity otherwise;  $f_p = f_p(\mathbf{e}'_p : \mathbf{e}'_p)$  is a function of the second invariant of the plastic strain rate deviator. All the functions introduced are nonnegative. The constitutive relations have the form

$$\eta = \eta_C = -\frac{\partial \varphi_1}{\partial T} - h_1 [(\epsilon' - \epsilon'_p) : (\epsilon' - \epsilon'_p)] \frac{1}{\rho} \frac{\partial \mu}{\partial T}, \quad \boldsymbol{\sigma} = \boldsymbol{\sigma}_C = -p \mathbf{I} + 2\mu(\epsilon' - \epsilon'_p), \quad p = \rho^2 \frac{\partial \varphi}{\partial \rho},$$

$$\mathbf{e}'_p = H \left( \boldsymbol{\sigma}' : \boldsymbol{\sigma}' - \frac{k_p^2 f_p^2}{\mathbf{e}'_p : \mathbf{e}'_p} \right) \left( \frac{k_p f_p}{\mathbf{e}'_p : \mathbf{e}'_p} \right)^{-1} \boldsymbol{\sigma}', \quad \mathbf{q} = k_q \nabla T, \quad U = U_C = \varphi - T \frac{\partial \varphi}{\partial T}.$$

The plasticity condition is implied by these relations and has the form

$$\boldsymbol{\sigma}' : \boldsymbol{\sigma}' = \left( \frac{k_p f_p}{\mathbf{e}'_p : \mathbf{e}'_p} \right)^2 (\mathbf{e}'_p : \mathbf{e}'_p).$$

An elastic-plastic medium corresponds to the homogeneous function of degree 1, i.e.,  $f_p = (\mathbf{e}'_p : \mathbf{e}'_p)^{1/2}$ . In this case the plasticity conditions are independent of the plastic strain rate, i.e., we have  $\boldsymbol{\sigma}' : \boldsymbol{\sigma}' = k_p^2$ .

**5.** Consider models of media subject to damage. We will regard the fracture as a process of accumulation of microdefects characterized by a special structural parameter  $\theta$  measuring damage. Without discussing details of possible physical definitions for damage (see, e.g., [16, 17]), we will establish the form of the constitutive relations suggested by the laws of thermodynamics.

5.1. Consider a modification of the model of the elastoviscoplastic medium. We assume that the damage increases if a fracture criterion  $\Phi(T, \epsilon, \epsilon_p, \theta) \geq 0$  is satisfied.

It is well known that the rigidity of the medium, as well as the velocity of propagation of waves in this medium, decrease as damage accumulates [13]. For this reason, we assume that the elastic moduli and the yield stress depend on the damage parameter and are expressed as

$$\mu = \mu_0(T)g_\mu(\theta), \quad K = K_0(T)g_K(\theta), \quad k_p = k_{p0}(T)g_p(\theta),$$

where  $K_0 = K_0(T)$  and  $\mu_0 = \mu_0(T)$  are the elastic moduli;  $k_{p0} = k_{p0}(T, \epsilon, \epsilon_p)$  is the yield stress for the undamaged medium. The functions  $g_\mu$ ,  $g_K$ , and  $g_p$  reflect the dependence of the corresponding quantities on the damage parameter and have the following properties:

$$0 < g_\mu, g_K, g_p \leq 1, \quad g_\mu(0) = g_K(0) = g_p(0) = 1, \quad g_\mu(\infty) = g_K(\infty) = g_p(\infty) = 0, \quad \frac{dg_\mu}{d\theta} \leq 0, \quad \frac{dg_K}{d\theta} \leq 0, \quad \frac{dg_p}{d\theta} \leq 0.$$

This implies that the strength of the medium decreases as the damage parameter increases.

For the free energy and the dissipation rate we have the simple expressions

$$\varphi = \frac{K}{2\rho_0} \left( \ln \frac{\rho}{\rho_0} \right) + \frac{\mu}{\rho_0} (\epsilon' - \epsilon'_p)^2 : \mathbf{I}, \quad D = H(\sigma' : \sigma' - k_p^2) k_p (\mathbf{e}' : \mathbf{e}')^{1/2} + \frac{k_q}{T} \nabla T \cdot \nabla T + H(\Phi) k_\theta \left( \frac{d\theta}{dt} \right)^2,$$

where  $k_q$  and  $k_\theta$  are nonnegative functions of  $T$ ,  $\epsilon$ ,  $\epsilon_p$ , and  $\theta$ . Using the general relations of (3.5) and neglecting the terms of higher order of smallness, we arrive at the following constitutive relations:

$$\eta = -\frac{\partial \varphi}{\partial T}, \quad \sigma = -p\mathbf{I} + \sigma', \quad p = K \frac{\rho}{\rho_0} \ln \frac{\rho}{\rho_0}, \quad \sigma' = 2\mu(\epsilon' - \epsilon'_p),$$

$$\mathbf{e}'_p = H(\sigma' : \sigma' - k_p^2) \left[ \frac{k_p}{(\mathbf{e}'_p : \mathbf{e}'_p)^{1/2}} \right]^{-1} \sigma', \quad \mathbf{q} = k_q \nabla T, \quad U = \varphi - T \frac{\partial \varphi}{\partial T}, \quad \frac{d\theta}{dt} = -\frac{H(\Phi)}{k_\theta(T, \epsilon, \epsilon_p, \theta)} \frac{\partial \varphi}{\partial \theta}.$$

These relations have been successfully used for the numerical simulation of the processes of fracture and strain localization [17].

5.2. We will give now the thermodynamic derivation of another model of fracture suggested in [16] to describe the behavior of geomaterials. In accordance with the experimental data for the majority of isotropic geomaterials, we assume that the free energy can be represented with a reasonably high degree of accuracy by a quadratic form of the elastic stain tensor (the difference of the strain tensor and the plastic strain tensor), with the coefficients depending on the damage parameter. With reference to the observation that geomaterials are plastically compressible, we take into account the dependence of the dissipation rate on the spherical component of the plastic strain tensor.

The expressions for the free energy and the dissipation rate occurring in the constitutive relations of the fracture model [16] have the form

$$\varphi = \frac{K(T, \theta)}{2\rho} [(\epsilon - \epsilon_p) : \mathbf{I}]^2 + \frac{\mu(T, \theta)}{\rho} (\epsilon' - \epsilon'_p)^2 : \mathbf{I},$$

$$D = \frac{K}{\Lambda \Theta} (\mathbf{e}_p : \mathbf{I})^2 + 2\mu\tau \mathbf{e}'_p : \mathbf{e}'_p + \frac{Q}{\Theta} \left( \frac{d\theta}{dt} \right)^2 + \frac{k_q}{T} \nabla T \cdot \nabla T,$$

$$Q = - \left[ \frac{1}{2} \frac{\partial K}{\partial \theta} ((\epsilon - \epsilon_p) : \mathbf{I})^2 + \frac{\partial \mu}{\partial \theta} (\epsilon' - \epsilon'_p)^2 : \mathbf{I} \right],$$

where  $\tau$  is the relaxation time,  $\Theta \geq 0$  is the rate of accumulation of damage,  $\Lambda \geq 0$  is the dilatancy rate, and  $k_q$  is the heat conductivity coefficient. The variables  $\tau$ ,  $\Theta$ ,  $\Lambda$ , and  $k_q$  are functions of the elastic strain tensor, damage, and temperature. The constitutive relations have the form

$$\eta = -\frac{\partial \varphi}{\partial T}, \quad \sigma = K\mathbf{I} : (\epsilon - \epsilon_p)\mathbf{I} + 2\mu(\epsilon' - \epsilon'_p), \quad \mathbf{e}'_p = \frac{\sigma'}{2\mu\tau}, \quad \mathbf{e}_p : \mathbf{I} = \frac{\Lambda\Theta}{K} \sigma : \mathbf{I},$$

$$\frac{d\theta}{dt} = \Theta(T, \epsilon - \epsilon_p, \theta), \quad \mathbf{q} = k_q \nabla T, \quad U = \varphi - T \frac{\partial \varphi}{\partial T}.$$

These constitutive relations have been utilized for the numerical simulation of the localization and fracture processes under dynamic and quasistatic loading [16–18].

6. We will show how one can modify a model of a porous material subject to fracture to take into account the sintering (consolidation) processes in a continuous medium. To that end, it is convenient to introduce a structural parameter depending on the plastic strain, the porosity  $\omega$ . The pore density is defined as the ratio of the volume of pores to the total volume occupied by the medium. The residual porosity corresponds to the unloaded state, i.e., to the

state with zero value of conservative stresses, and can be calculated by using either the porosity  $\omega$  or in terms of the plastic strain. We have

$$\rho_p = \rho_{\max}(1 - \omega), \quad \frac{d\rho_p}{dt} = -\rho_p(\mathbf{e}_p : \mathbf{I}). \quad (6.1)$$

The porosity and the volumetric plastic strain are related by

$$\mathbf{e}_p : \mathbf{I} = \frac{1}{1 - \omega} \frac{d\omega}{dt}. \quad (6.2)$$

The definition of the porosity implies that  $0 \leq \omega \leq \omega_{\max} < 1$ , where  $\omega_{\max}$  is the maximum value of the porosity beyond which the medium falls apart into separate particles. The equality  $\omega = \omega_{\max}$  may take place, for example, for the initial state of a composite medium having the form of a powder of several components filling a mould. The value of  $\omega_{\max}$  can be readily calculated by using the densities of the components, their percentage and initial volume. If the pores are wetted with liquid (melted) components, capillary forces may act on the pore surfaces. The pores, whose surfaces are acted upon by capillary forces, are referred as active pores. The active pores may cause sintering (consolidation) effect in the medium. To describe this effect, one should take into account the free energy of the active pores in the expression for the free energy of the continuous medium,  $\varphi_\omega(T, \omega)$ . The models of Section 5 being modified in such a way lead to the following expressions for the free energy and the dissipation rate:

$$\begin{aligned} \varphi &= \frac{K}{2\rho_0} \left( \ln \frac{\rho}{\rho_p} \right)^2 + \frac{\mu}{2\rho} (\boldsymbol{\epsilon}' - \boldsymbol{\epsilon}'_p)^2 : \mathbf{I} + H(T - T_m) \varphi_\omega(T - T_m, \omega), \\ D &= \frac{1}{\lambda_p} (\mathbf{e}'_p : \mathbf{e}'_p)^2 + \frac{k_q}{T} \nabla T \cdot \nabla T + \frac{H(\omega)}{\lambda_\omega} \left( \frac{d\omega}{dt} \right)^2 + \frac{H(\Phi)}{\lambda_\theta} \left( \frac{d\theta}{dt} \right)^2, \end{aligned}$$

where  $\lambda_p$ ,  $k_q$ ,  $\lambda_\omega$ , and  $\lambda_\theta$  are nonnegative functions of  $T$ ,  $\boldsymbol{\epsilon}$ ,  $\boldsymbol{\epsilon}_p$ ,  $\omega$ , and  $\theta$ . The quantity  $T_m$  identifies the melting temperature at which the pores become active. The constitutive relations have the form

$$\begin{aligned} \eta &= -\frac{\partial \varphi}{\partial T}, \quad \boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\sigma}', \quad p = K \frac{\rho}{\rho_0} \ln \frac{\rho}{\rho_p}, \quad \boldsymbol{\sigma}' = 2\mu(\boldsymbol{\epsilon}' - \boldsymbol{\epsilon}'_p), \\ \boldsymbol{\epsilon}'_p &= \lambda_p \boldsymbol{\sigma}', \quad \mathbf{q} = k_q \nabla T, \quad U = \varphi - T \frac{\partial \varphi}{\partial T}, \quad s_\omega = \rho \frac{\partial \varphi_\omega}{\partial \omega} (1 - \omega), \\ \frac{d\omega}{dt} &= -H(\omega) \frac{\lambda_\omega(\pi^{(1)})}{1 - \omega} (p + s_\omega), \quad \frac{d\theta}{dt} = -H(\Phi) \lambda_\theta(\pi^{(1)}) (\varphi - \varphi_\omega), \end{aligned}$$

where  $s_\omega$  is the ‘‘sintering stress’’ [21, 22]. The sintering stress and the free energy of pores are nonnegative. The sintering stress leads to the consolidation effect in the material only if the pores are active, i.e.,  $T \geq T_m$ . The sintering stress does not obey the equilibrium conditions. It represents capillary forces acting on the surfaces of pores. The yield stress and the elastic moduli in the model in question are functions of damage and porosity. These functions tend to zero as  $\theta \rightarrow \infty$ ,  $\omega \rightarrow 1$ , and tend to their values for the solid material as  $\theta \rightarrow 0$ ,  $\omega \rightarrow 0$ . Both the structural parameters, porosity and damage, obey evolution-type constitutive relations. The porosity is related to the volumetric plastic strain and can be decreased under the action of the external pressure (cold pressing) and/or the sintering stress (hot sintering). The relations derived resemble those of [22] presented for sintering processes. We have shown the connection of sintering theory with the laws of thermodynamics and have given a thermodynamic interpretation of the sintering stress. This theory has been used in calculations and shows promising results as regards the prediction of the shape and porosity distribution for bodies subjected to compaction.

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