DESCRIPTION OF GRANULAR
MATERIALS BY MEAN VALUES

Ondřej Navrátil

Institute of Rock Structure and Mechanics, Academy of Sciences of Czech Republic,
V Holešovičkách 41, 182 09 Prague 8, Czech Republic

ABSTRACT. The author explains, in this paper, that if the average values of density, velocity, stress tensor, etc. are adequately defined for granular materials,these average quantities fulfill the continuum mechanics equations. On the other hand, such an averaging does not yield constitutive relations, which have to be specified empirically. It is also shown that the method known from thermodynamics cannot be used to define, for granular materials, the state functions, such as the absolute temperature and entropy.

KEY WORDS: continuum mechanics, granular materials, thermodynamics.

1. INTRODUCTION

In the nature, there occur frequently materials, which can very well be approximated by a granular material consisting of individual particles, grains, which themselves behave as a continuum. The description of such material by describing the behaviour of individual grains, the microscopic description, is practically unfeasible, because a large number of equations of motion had to be solved for individual grains and, in addition to that, we would have to know the initial and boundary conditions. The description of a granular material is therefore approximated by continuum mechanics; I shall denote this procedure, for granular materials, as the macroscopic theory. In this paper, I want to deal with the problem, how the microscopic quantities (quantities describing individual grains) are related to the macroscopic ones (quantities describing the material as a whole). The macroscopic quantities will be defined as certain mean values of the microscopic quantities so to satisfy the motion equations known from continuum mechanics, i.e. the equation of continuity, equation of conservation of momentum, equation of conservation of moment of momentum and equation of conservation of energy.

In order to get, in continuum mechanics, a closed system of equations, we should also set the constitutive relations. However, the used method of definition of macroscopic quantities does not give constitutive relations. We must therefore determine them empirically instead of finding them from relations between macroscopic and microscopic quantities. Thermodynamics (Truesdell, 1984) plays an important role in the theory of constitutive relations. I will show that, for granular materials, it is impossible to introduce, as state function in the way known from thermodynamics

(e.g. Kvasnica, 1965), the entropy and the absolute temperature. In order to construct, for granular materials, a theory similar to thermodynamics, we must accept the statistical description of granular materials. However, such a description differs in principle from the deterministic description, used in this paper. Nevertheless, I think that the statistical description of the granular material is the only one that can yield both the equations of motions and constitutive relations.

2. Equations describing the movement of individual grains

Individual grains, B_a, will be described by Lagrange's coordinates Σ_a and the grain boundary will be denoted by S_a. Let the motion of grain be defined by C^∞ mapping $\chi_a : B_a \times \mathbb{R} \to \mathbb{R}^3$, which I will write as

$$\xi^i = \chi_a^i(\Sigma_a, t). \tag{2.1}$$

It is assumed, for this mapping, that there exists, for each $t \in \mathbb{R}$, an inverse mapping χ_{at}^{-1}, which is also infinitely differentiable. In fact, the mapping χ_a determines the position of the point Σ_a of the grain B_a at time t.

For each grain B_a, I define the deformation gradient $F_{ak}^i(\Sigma_a, t)$ by relation

$$F_{ak}^i(\Sigma_a, t) = \frac{\partial \chi_a^i}{\partial \Sigma_a^k}(\Sigma_a, t), \tag{2.2}$$

for which $J_a = \det F_a \neq 0$ holds true. It results from the continuity F_a that the coordinates Σ_a can be chosen in the way to satisfy always $J_a > 0$. Such a choice of coordinates will be assumed herein after.

Further, I define the velocity of motion for each grain B_a by the relation

$$\bar{v}_a^i(\Sigma_a, t) = \frac{\partial \chi_a^i}{\partial t}(\Sigma_a, t) \qquad resp. \qquad v_a^i = \bar{v}_a^i \circ \chi_{at}^{-1}. \tag{2.3}$$

Similarly, I define the acceleration as

$$\bar{a}_a^i(\Sigma_a, t) = \frac{\partial \bar{v}_a^i}{\partial t}(\Sigma_a, t) \qquad resp. \qquad a_a^i = \bar{a}_a^i \circ \chi_{at}^{-1}. \tag{2.4}$$

It is then evident that it holds

$$a_a^i = \dot{v}_a^i = \frac{\partial v_a^i}{\partial t} + \frac{\partial v_a^i}{\partial \xi^k} v_a^k, \tag{2.5}$$

where I use the summation convention and the dot over the v denotes here after the material derivation.

Further, the density $\rho_a(\xi, t)$ is defined, which is related to the density $\tilde{\rho}_a(\Sigma_a)$ in Lagrange's coordinates by

$$\rho_a = (\tilde{\rho}_a J_a^{-1}) \circ \chi_{at}^{-1}. \tag{2.6}$$

It is evident, from this definition, that the density of grain B_a at time t can differ from zero only for $\xi \in \chi_{at}(B_a) = B_a(t)$. Further on, I will use the convention that all quantities related to grain B_a have at the time t a support, which is a subset of $B_a(t)$. Thus, I define them by zero except for $B_a(t)$. This convention will be used even for the velocity v_a^i and the acceleration a_a^i.

A consequence of the fact that $\tilde{\rho}$ is a function only the coordinates Σ_a and not of the time and of (2.6), is the equation of continuity. This equation is an expression of the mass balance and has the form

$$\frac{\partial \rho_a}{\partial t} + \frac{\partial(\rho_a v_a^k)}{\partial \xi^k} = 0. \tag{2.7}$$

This equation as well as the other equations in this Section have to be understood as equations of generalized functions. That means that is holds, for each function $\varphi \in C_0^\infty(\mathbb{R}^4)$, i.e. an infinitely differentiable function with a compact support

$$-\int_{\mathbb{R}^4} \rho_a(\xi, t) \left[\frac{\partial \varphi}{\partial t} + \frac{\partial \varphi}{\partial \xi^k} v_a^k \right] d^3\xi \, dt = 0.$$

The validity of this equation is easily verified, if, instead of ξ^k the value of Σ_a^k defined by (2.1) and (2.6) is used and the independence of the integration range on time t is introduced.

The law of conservation of momentum can be expressed, by distribution equations, as

$$\frac{\partial \rho_a v_a^i}{\partial t} + \frac{\partial \rho_a v_a^i v_a^k}{\partial \xi^k} = \rho_a b^i + \frac{\partial T_a^{ik}}{\partial \xi^k} + f_a^i \delta_{S_a}, \tag{2.8}$$

where b^i is the density of external body force per unit mass, T^{ik} is the stress tensor within the grain $B_a(t)$ and f_a^i is the surface density of external force affecting the grain $B_a(t)$, whose support is limited to the boundary $S_a(t)$ of this grain. This equation involves both the motion equations within the grain and the boundary conditions given by the distribution of forces on the grain surface. The validity of this equation is checked, similarly as for (2.7), by transition to Lagrange's coordinates.

The law of conservation of the angular momentum for the grain B_a gives the condition of symmetry of the stress tensor, i.e.

$$T_a^{ik} = T_a^{ki}. \tag{2.9}$$

Another of the pertinent and generally valid physical law is the energy balance law. Considering the heat flow and thermal sources, the law of conservation of energy for the grain B_a acquires the form of

$$\frac{\partial \rho_a E_a}{\partial t} + \frac{\partial \rho_a E_a v_a^k}{\partial \xi^k} =$$

$$= \rho_a b_a^i v_a^i + \frac{\partial T_a^{ik} v_a^i}{\partial \xi^k} + f_a^i v_a^i \delta_{S_a} + \rho_a r_a - \frac{\partial h_a^k}{\partial \xi^k} + \sigma_a \delta_{S_a}, \tag{2.10}$$

7

where E_a is the density of total grain energy per unit mass, r_a is the density of thermal sources in $B_a(t)$ per units mass and time, σ_a is the surface density of thermal sources per unit time, and h_a^k is the heat flux vector in the grain. When the density of internal energy is introduced by relation $\varepsilon_a = E_a - \frac{1}{2}v_a^i v_a^i$ and (2-7)–(2.10) are applied, the following equations are obtained

$$\frac{\partial(\rho_a \varepsilon_a)}{\partial t} + \frac{\partial(\rho_a \varepsilon_a v_a^k)}{\partial \xi^k} = T_a^{ik} L_{aik} + \rho_a r_a - \frac{\partial h_a^k}{\partial \xi^k} + \sigma_a \delta_{S_a} , \qquad (2.11)$$

where

$$L_{aik} = \frac{1}{2}\left[\frac{\partial v_a^i}{\partial \xi^k} + \frac{\partial v_a^k}{\partial \xi^i}\right] . \qquad (2.12)$$

Finally the Clausius–Duhem inequality should hold for each $B_a(t)$ grain, which expresses, in continuum mechanics, the second thermodynamic law, i.e.

$$\frac{\partial(\rho_a \eta_a)}{\partial t} + \frac{\partial(\rho_a \eta_a v_a^k)}{\partial \xi^k} + \frac{\partial(h_a^k/\theta_a)}{\partial \xi^k} - \frac{\rho_a r_a}{\theta_a} - \frac{\sigma_a}{\theta_a}\delta_{S_a} \geq 0, \qquad (2.13)$$

where η_a is the entropy per unit mass in the $B_a(t)$ grain and $\theta_a > 0$ is the absolute temperature. The inequality (2.13) means that, if the left side is applied to a non-negative function from C_0^∞, a non-negative number is obtained.

As generally known, constitutive relations are to be added to these equations. How limited the constitutive relations are, is illustrated, e.g., by rational thermodynamics (Truesdell, 1984). I will not discuss here these constitutive relations, but I will assume that if b^i, r_a, f_a^i and σ_a are given as functions of ξ^k and t and functions $\tilde{\rho}_a$, $\chi_a^i(\Sigma_a, t_0)$, $v_a^i(\xi, t_0)$ and $\theta(\xi, t_0)$, the motion of the grain B_a and the temperature distribution in that grain are unambiguously determined for $t \geq t_0$.

3. Equations describing the motion of a system of particles

Considering now the system of more particles, equations discussed in Section 2 must hold for each individual grain. In addition to these equations, the grain motion must also satisfy further conditions, which result from bonds between individual grains. I will assume that motion takes place within the area limited by surface S_0. The surface S_0 should be defined more precisely by the equation $\psi(\xi, t) = 0$ and the motion should take place within the area $\psi(\xi, t) \leq 0$. In such a case, the function should satisfy, in addition to equations quoted in Section 2, the relations, which guarantee that the grain motion takes place within the area limited by the surface $S_0(t)$ and that the grains do not penetrate each other. It should therefore hold, for each grain primarily that $\psi(\chi_a(\Sigma_a, t), t) \leq 0$. Moreover, the points for which the equality holds, must fall to the boundary $S_a(t)$. If $S_{a0}(t) = S_a(t) \cap S_0(t)$ is denoted, it must hold, for these points

$$(v_a^i - v_0^i)n_{a0}^i \leq 0 \quad , \qquad (3.1)$$

where v_0^i is the velocity of motion a point of the surface $S_0(t)$ and n_{a0}^i is the vector of external normal to the surface of grain $B_a(t)$ at the contact point with the surface $S_0(t)$. Let the forces acting on this grain on the contact surface $S_{a0}(t)$ are denoted by f_{a0}^i. Similarly, let the thermal sources are denoted by σ_{a0}.

Since the grains do not penetrate each other, it should hold, for $a \neq b$,

$$B_a(t) \cap B_b(t) = S_a(t) \cap S_b(t) = S_{ab}(t). \tag{3.2}$$

Moreover, it must hold for all point from $S_{ab}(t)$

$$(v_a^i - v_b^i) n_{ab}^i \leq 0, \tag{3.3}$$

where n_{ab}^i is the external normal to the surface $S_a(t)$. Let the forces acting on this boundary of the grain $B_a(t)$ are denoted by f_{ab}^i and the thermal sources by σ_{ab}. Then the surface force on the grain $B_a(t)$ will be given by the relation

$$f_a^i \delta_{S_a} = \sum_{b \neq a} f_{ab}^i \delta_{S_{ab}} + f_{a0}^i \delta_{S_{a0}} \tag{3.4}$$

and the surface thermal sources for this grain are

$$\sigma_a \delta_{S_a} = \sum_{b \neq a} \sigma_{ab} \delta_{S_{ab}} + \sigma_{a0} \delta_{S_{a0}}. \tag{3.5}$$

If on the contact face of two grains S_{ab} there are no other surface forces acting except the mutual forces between B_a and B_b (for example there does not exist any surface tension), it must hold that

$$f_{ab}^i + f_{ba}^i = 0, \tag{3.6}$$

which is the Newton's third law of motion. Similarly, if the thermal sources on the surface are caused exclusively by the mechanical force f_{ab}^i, the expression

$$\sigma_{ab} + \sigma_{ba} = 0 \tag{3.7}$$

must hold. However, for the description of the whole system, the forces f_{ab} and the thermal sources σ_{ab} have generally to be specified by constitutive relations.

We shall now assume that the constitutive relations are expressed by means of functions χ_a^i, v_a^i and θ_a or, eventually, by their derivations. It is further assumed that, if there are specified the motion of limiting surface $S_0(t)$, temperature distribution $\theta_0(t)$ on this surface, density of external forces b^i, intensity of external thermal sources r_a and initial state of all grains, i.e. $\chi_a^i(\Sigma_a, t_0)$, $v_a^i(\xi, t_0)$ and $\theta_a(\xi, t_0)$, the motion of all grains for $t > t_0$ and the temperature distribution within these grains are unambiguously determined.

9

As it has been already noted in the Introduction, the states of individual grains are usually unaccessible to experimental measurements. We are, in fact, measuring only certain mean values of corresponding quantities. I am defining, in this Section, mean values by means of convolution with a certain non-negative function, whose integral equals to one. I can use, in principle, any non-negative function, such one with existing needed integrals. Here, I will use a function from $C_0^\infty(\mathbb{R}^4)$ in order to get infinitely differentiable functions. If we use a function with a lower number of derivations, we would get, of course, functions with less derivations. One such case is quoted in (Drew, 1971). Another possibility is to use the convolution with a spatial function only, which may be adequate if the considered functions are sufficiently continuous functions of time.

Let the function $\varphi \in C_0^\infty(\mathbb{R}^4)$ be given such that $\varphi \geq 0$ and

$$\int_{\mathbb{R}^4} \varphi(x,t)\, d^3x\, dt = 1\,.$$

Let the bounded functions $F_a(x,t)$ be given, which are measurable in Lebesquian sense and let

$$F_{at} = F_a(.,t) : \mathbb{R}^3 \to \mathbb{R}$$

be defined. Then, it holds for each $t \in \mathbb{R}$ that the $supp(F_{at}) \subset B_a(t)$. Then I define

$$< F > (x,t) = \sum_a \int_{\mathbb{R}^4} F_a(\xi,\tau)\,\varphi(x-\xi, t-\tau)\, d^3\xi\, d\tau\,. \tag{4.1}$$

Functions thus defined are, for a fixed t, from $C_0^\infty(\mathbb{R}^3)$ and as functions of all four variables they are infinitely differentiable.

First, the mean density ρ is defined by relation

$$\rho(x,t) = < \rho > (x,t) \tag{4.2}$$

and for all (x,t), where $\rho(x,t) \neq 0$, the mean velocity V^i by

$$\rho V^i(x,t) = < \rho v^i > (x,t)\,. \tag{4.3}$$

The mean velocity V^i is not defined in points with zero density. Outside the support ρ it may be defined by zero. However, it is, in general, impossible to define additionally the functions V^i at the boundary of $supp(\rho)$ so as to be continuous. Nevertheless, as the velocities v_a^i are bounded for each a, there is on $int(supp(\rho))$ also a bounded V^i, because

$$|\rho V^i| = \left| \sum_a \int_{\mathbb{R}^4} \rho_a v_a^i(\xi,\tau)\,\varphi(x-\xi,t-\tau)\, d^3\xi\, d\tau \right| \leq$$

$$\leq \sum_a \int_{\mathbb{R}^4} \rho_a |v_a^i(\xi,\tau)|\,\varphi(x-\xi,t-\tau)\, d^3\xi\, d\tau \leq K\rho\,.$$

Moreover, it is evident from the definition of V^i that it is infinitely differentiable on this set. If we confine ourselves to this set, then the equation of continuity

$$\dot{\rho} + \rho \frac{\partial V^k}{\partial x^k} = 0 \tag{4.4}$$

must hold. This is evident from (2.7), when we multiply this equation by the function $\varphi(x - \xi, t - \tau)$, integrate and sum it up over a.

When the same procedure is applied to (2.8)

$$\rho \dot{V}^i = \rho B^i + \frac{\partial T^{ik}}{\partial x^k} + F^i \tag{4.5}$$

results, where

$$\rho B^i = < \rho b^i >, \tag{4.6}$$

$$F^i = < f^i \delta_S > \tag{4.7}$$

and

$$T^{ik} = < T^{ik} - \rho v^i v^k > - \rho V^i V^k = < T^{ik} - \rho u^i u^k >, \tag{4.8}$$

where we introduced the relative velocity u_a^i by

$$u_a^i = v_a^i(\xi, \tau) - V^i(x, t). \tag{4.9}$$

Using (3.4) it is possible to write the (4.7) in a more suitable form as

$$F^i = \sum_a \int_{\mathbb{R}^4} \left[\sum_{b \neq a} (f_{ab}^i \delta_{S_{ab}}(\xi, \tau) + f_{a0}^i \delta_{S_{a0}}(\xi, \tau) \right] d^3\xi \, d\tau = F_{int}^i + F_{ext}^i, \tag{4.10}$$

where

$$F_{int}^i = \frac{1}{2} \sum_{\substack{a,b \\ a \neq b}} \int_{\mathbb{R}^4} (f_{ab}^i + f_{ba}^i) \, \delta_{S_{ab}}(\xi, \tau) \varphi(x - \xi, t - \tau) \, d^3\xi \, d\tau$$

and

$$F_{ext}^i = \sum_a \int_{\mathbb{R}^4} f_{a0}^i \delta_{S_{a0}}(\xi, \tau) \, d^3\xi \, d\tau.$$

It is evident, from these definitions, that F_{ext}^i are forces by which the boundary S_0 affects the body's interior and F_{int}^i are internal forces. If (3.6) holds, F_{int}^i vanish, but if there is a surface tension between individual grains, this fact about F_{int}^i cannot be asserted a priori.

By averaging the (2.9) for angular momentum, the only result can be obtained that the stress tensor, defined in (4.8) is symmetrical, i.e.

$$T^{ik} = T^{ki}. \tag{4.11}$$

11

Rather than by direct averaging of the relation (2.11) for ε_a, then mean values of the density of internal energy will be defined as

$$\rho e = <\rho E> -\tfrac{1}{2}\rho V^i V^i =< \rho(\varepsilon + \tfrac{1}{2}v^i v^i)> -\tfrac{1}{2}\rho V^i V^i =< \rho(\varepsilon + \tfrac{1}{2}u^i u^i)> . \quad (4.12)$$

It can be seen from this relation, that also the kinetic energy of relative motion of individual grains is included into
relation can be obtained by averaging of relevant equations:

$$\rho \dot{e} = T^{ik} L_{ik} + \rho R + S - \frac{\partial H^k}{\partial x^k}, \quad (4.13)$$

where

$$\rho R =< \rho(b^i u^i + r)>, \quad (4.14)$$

$$S =< (f^i u^i + \sigma)\delta_S >, \quad (4.15)$$

$$H^k =< h^k + \rho \varepsilon u^k + \tfrac{1}{2}\rho u^i u^i u^k - T^{ik} u^i > \quad (4.16)$$

and

$$L_{ik} = \frac{1}{2}\left[\frac{\partial V^i}{\partial x^k} + \frac{\partial V^k}{\partial x^i}\right]. \quad (4.17)$$

Using the same procedure, which led from the equation (4.7) to (4.10), the expression

$$S = S_{int} + S_{ext} \quad (4.18)$$

is obtained, where

$$S_{int} = \sum_{\substack{a,b \\ a\neq b}} \int_{\mathbb{R}^4} \left[\tfrac{1}{4}(f^i_{ab} + f^i_{ba})(u^i_a + u^i_b) + \tfrac{1}{4}(f^i_{ab} - f_{ba})(u^i_a - u^i_b)+ \right.$$

$$\left. + \tfrac{1}{2}(\sigma_{ab} + \sigma_{ba})\right]\delta_{S_{ab}}\varphi\, d^3\xi\, d\tau$$

and

$$S_{ext} = \sum_{a} \int_{\mathbb{R}^4} (f^i_{a0}u^i_a + \sigma_{a0})\,\delta_{S_{a0}}(\xi,\tau)\,\varphi(x - \xi, t - \tau)\, d^3\xi\, d\tau .$$

These expression have the same interpretation as similar ones for force.

It is quite natural to expect that the inequality for mean entropy will be derived accordingly. However, that is not so. It is evident,though, that the inequality for quantity $\rho \eta =< \rho \eta >$ can be obtained by averaging, but it does not result from anywhere that the quantity η can be identified with the mean entropy of the entire system of grains. This may be seen, e.g. from the fact, that we cannot generally succeed to define, by similar averaging, the mean values of the absolute temperature of the system. The problem consists in the fact that the entropy is a quantity defined

12

for the entire set of systems and expresses the statistical properties of this set. For one system here discussed, the entropy is not defined at all. The same holds for the absolute temperature of the system. In order to be able to introduce these quantities, we have to investigate the thermodynamics of the system or describe the granular materials by means of statistics of the entire set of systems.

5. Relation to some constitutive models

In the preceding Section, the mean values of some interesting quantities have been defined for a granular material with the intention to develop similar motion equations to those holding for usual continuum. System of these equations has yet to be completed by constitutive relations, which, however, do not result from this theory. Obviously, the definition equations from preceding Section cannot be used as constitutive relations, even if we introduce into them constitutive relations for material of individual grain, which we consider known, since they are supposed interconnect the macroscopic variables, while the definition relations connect the macroscopic quantities with certain functions of microscopic variables. It is evident from the definition of macroscopic quantities that we would need to exclude, from definition equations, the mean values of microscopic quantities and thus obtain relations between macroscopic quantities only. However, this is generally impossible. In principle, new mean quantities can be defined with defined physical significance and it can be tried to use these quantities for obtaining constitutive relations. However, this procedure cannot be consider too promising, either. The author himself is considered that such theory cannot meet with results in the form of constitutive relations.

Unlike the usual motion equations for continuum, our motion equations include terms F_{int}^i and S_{int}, which characterize the interaction within the system of grains. These quantities do not depend on external fields and represent therefore the properties of material. They should be therefore specified by constitutive equations. The possibility is suggested to consider F_{int}^i the divergence of some tensor field A^{ik}, i.e. to assume

$$F_{int}^i = \frac{\partial A^{ik}}{\partial x^k} \qquad (5.1)$$

and define a new "stress" tensor by

$$\tilde{T}^{ik} = T^{ik} + A^{ik} . \qquad (5.2)$$

In such a case , the equation (4.5) will be transformed, within the body, into the usual equation of continuum mechanics and we could try to find the constitutive relations for $\tilde{T}^{ik}$. However, in such case the "stress" tensor $\tilde{T}^{ik}$ is not necessarily symmetric, because, as it results from (4.11), the law of conservation of the angular momentum requires only the symmetry of T^{ik}. The assumption of non-symmetry of the stress tensor appeared already in some formulation of the constitutive relations for geomaterials, but there, the non-symmetry is explained by force moment, originating from the rotation of individual grains. Such an approach differs, however, substantially from the author's concept. There can be put a general question,

13

whether there exists any choice of the "stress" tensor $\tilde{T}^{ik}$, which would be physically justifiable, i.e. whether there exists an experiment, which would decide, how to choose correctly an A^{ik} fulfilling (5.1) or whether it would not be more natural to determine constitutive relations for F^i_{int}.

Let us come back to the ambiguity of the stress tensor in (4.8). This is especially important in the case, when F^i_{int} vanishes, because, in such a case, the stress tensor plays the decisive part in (4.5). This happens when there isn't any surface tension between grains or when this term can be neglected, which will be a frequent case. Because only the divergence of the stress tensor is specified in the equation (4.5), it is possible to add to the stress tensor an arbitrary tensor A^{ik}, for which

$$\frac{\partial A^{ik}}{\partial x^k} = 0 \tag{5.3}$$

holds. It can be therefore chosen

$$\bar{T}^{ik} = T^{ik} + A^{ik}, \tag{5.4}$$

where A^{ik} fulfills the eq.(5.3). Even such a choice of the stress tensor can involve its non-symmetry. However, when the stress tensor form (5.4) is used in the equation for energy, we get

$$\rho \dot{e} = \bar{T}^{ik}\frac{\partial V^i}{\partial x^k} + \rho R + S - \frac{\partial \bar{H}^k}{\partial x^k}, \tag{5.5}$$

where

$$\bar{H}^k = < h^k + \rho \varepsilon u^k + \tfrac{1}{2}\rho u^i u^i u^k - T^{ik} u^i > + A^{ik} V^i. \tag{5.6}$$

It may be seen, from this relation, that in the choice of the stress tensor (5.4), the vector of the heat flux depends explicitly on the average velocity. As the heat flux vector is specified by a constitutive equation, the constitutive relations would have to be dependent, in such a case, on the velocity of the system. This is a dispute about the principle of objectivity of constitutive relations, which is required by rational thermodynamics. It will be therefore assumed that the mean stress tensor is defined by (4.8) and thus being symmetric.

It should also be noted that we did not at all define the strain tensor, which plays an important role in many constitutive models. This is caused by the fact that I use, for the description of the macroscopic system, Euler's coordinates and consequently, I choose, for the reference system, the instantaneous state of the body, where the strain tensor equals to identity. Also another reference system could, of course, be defined, but this would result only in another equivalent description of the system. In granular materials there does not exist any physically relevant reference system with permanent zero stress as for the elastic materials. It is therefore more natural to look out, for granular materials, for incremental constitutive equations. It would be interesting to compare how the otherwise suggested constitutive incremental equations for granular materials agree with definition equations of this theory. To

this purpose, the time derivation of the stress tensor from the equation (4.8) should be carried out. After long algebra, the following equation is obtained

$$\dot{T}^{ik} + T^{ik}V^r_{,r} + T^{ir}V^k_{,r} + T^{kr}V^i_{,r} =$$
$$= - <\rho\,(b^i u^k + b^k u^i)> - <(f^i u^k + f^k u^i)\,\delta_S> +$$
$$+ \frac{\partial}{\partial x^k} <\rho u^i u^k u^r - T^{ik}u^r - T^{ir}u^k - T^{kr}u^i> +$$
$$+ <\dot{T}^{ik} + T^{ik}u^r_{,r} + T^{ir}u^k_{,r} + T^{kr}u^i_{,r}> . \quad (5.7)$$

However, computation – compared with constitutive method – is so intricate, that no reasonable results could be obtained.

Another very similar theory is the theory of multicomponent mixtures, known from rational thermodynamics (Truesdell, 1984). It can be seen easily that the derivation of motion equations in this theory and in the theory of mixtures is very similar. The multicomponent mixture introduces, additionally, the material ratio Φ_A for each individual component A. In our theory the following expression corresponds with this ratio

$$\Phi_A(x,t) = <\nu_A> = \sum_{a \in A} \int_{\mathbb{R}^4} \nu_a(\xi,\tau)\,\varphi(x-\xi, t-\tau)\,d^3\xi\,d\tau\,, \quad (5.8)$$

where ν_a is the characteristic function of the set $B_a(t)$ and A is the set of all such instances, where the grain B_a belongs into the component A. However, the theory of mixtures assumes that for functions Φ_A equations of motion hold true, which have the form similar to laws of conservation. When the material derivation (5.8) is carried out, the expression

$$\dot{\Phi}_A = <u^k_A n^k_A \delta_{S_A}> \quad (5.9)$$

is obtained. Generally it is not possible to give to this equation the significance of a balance equation. In fact, such an assumption is again a constitutive relation. Such assumption is used for derivations of constitutive relations for granular materials in (Goodman and Cowin, 1972). Moreover, the existence of entropy is assumed in this paper, as well as, from the second thermodynamic principle, the Duhem-Clausius inequality, the limiting conditions for constitutive relations are derived, as it is usual in rational thermodynamics. As it has been noted before, the entropy cannot be defined simply by averaging the microscopic equations. Even the thermodynamic axioms themselves do not guarantee the existence of entropy and it remains therefore a question, whether the entropy can be introduced for granular materials at all. This problem is discussed in the following Section.

6. GRANULAR MATERIALS AND THERMODYNAMICS

In this part, the procedure, which leads, in thermodynamics to the definition of absolute temperature and entropy, will be applied to granular materials. The

procedure is described in (Kvasnica, 1965). It is assumed, in thermodynamics, that the state of a system is determined by the entirety of all external conditions, in which the studied system occurs, and by the entirety of its independent properties. Thus, it is assumed that the state of a system is determined by the entirety of all its external and the independent internal parameters. Obviously, the number of external and independent internal parameters has to be assessed, for given system, empirically.

The first thermodynamics axiom: Each macroscopic system, which appears, since a certain moment $t = t_0$ at given temporally constant external conditions unavoidably attains the so-called state of thermodynamic equilibrium, where macroscopic processes and changes do not exist any longer. At the state of thermodynamic equilibrium, all state parameters have constant values. Whatever additional change of the macroscopic state, after formation of thermodynamic equilibrium, is possible only by a new external intervention. Let this axiom be considered well checked experimentally also for granular materials.

A thermally homogeneous system at the state of thermodynamic equilibrium will be investigated now. It should be noticed that as a thermally homogeneous system such a system is considered, where there do not exist any adiabatically isolated parts and a heat exchanges between whatever parts of the system is thus possible. The second thermodynamics axiom reads as follow: The state of thermodynamic equilibrium of the thermally homogeneous system is unambiguously determined by set of external and one internal parameter, for which the energy of system may be chosen. All others parameters of this system can be expressed as functions of external parameters and energy of the system. This axiom enables to us introduce, in a thermally homogeneous system at the state of thermodynamic equilibrium, an experimental temperature and the second thermodynamic axiom to be formulated as follow: At the state of thermodynamic equilibrium of a thermally homogeneous system all internal parameters are functions of external parameters and temperature of this system.

In order to satisfy this axiom for granular materials, a sufficient number of external parameters must be chosen to distinguish various systems at the state of thermodynamic equilibrium. The following external parameters will be considered: shape of the limiting surface S_0, external force field b^i, in a N–component system, the density of individual components ρ_A and $N-1$ material ratios Φ_A. Let us assume that the state of a thermally homogeneous system at the state of thermodynamics equilibrium is unambiguously determined by the temperature and these parameters.

From the thermodynamic viewpoint the quasistatic processes are important, i.e. processes leaving the system at any moment in the state of thermodynamic equilibrium. The state of such a system is unambiguously determined, according to the second thermodynamic axiom, by instantaneous values of its external parameters and temperature. It is usually assumed that the external parameters and temperature of the system can be changed arbitrary in the neighbourhood of each state point and thus, the quasistatic processes are also reversible ones. For a thermally homogeneous system at the state of thermodynamic equilibrium, the existence of absolute

16

temperature as an integrating factor of the differential form dQ and existence of the state function, entropy, can be derived from the above-mentioned property of quasistatic processes and from the Caratheorory's formulation of the second thermodynamic principle. In fact, the second thermodynamic principle for quasistatic process is reduced, in this case, to the existence of these two state functions.

However, external parameters and the temperature of the quasistatic process cannot be changed arbitrary in granular materials. This can be seen, for example, from the experiment with the compression of sand: the sand in a vessel can be compressed, but not expanded. Consequently, for granular materials, the second thermodynamic principle does not result in the existence of an integration factor of differential form dQ, and thus neither of temperature and entropy. It is impossible, for granular materials, to reduce the second thermodynamic principle for reversible processes to existence of absolute temperature and entropy of the system. This is the reason, why the procedure known from rational thermodynamics, which leads to restriction of constitutive relations and which still uses the entropy, is virtually useless for granular materials.

7. CONCLUSION

The method of averaging, used in this paper, is very simple and should only prove that the description of granular materials by mean values can be transformed into a form, very similar to the description of continuum. Moreover, it explains, which constitutive relations in the theory have to be specified from experiments. However, it is quite obvious that this theory cannot yield constitutive relations because, when specifying the macroscopic variables, the microscopic systems corresponding to the same values of macroscopic variables, can develop differently. It would be therefore more adequate, even if much more difficult, to approach the problem of description of granular materials statistically. This would mean not to investigate a single microscopic system, as it has been done here, but the entire set of microscopic systems with similar macroscopic properties. To this purpose, it would be, of course, necessary to define adequately the probability space and investigate, within it, the distribution of probability. The fact that we did not succeed to define the entropy in the same way as in thermodynamics, proves, that the distribution of probability will not be so simple as in thermodynamics. However, I am convinced that only such a statistical description could yield not only macroscopic equations of motion, but also constitutive relations for granular materials.

REFERENCES

Drew D.A. (1971), *Averaged Field Equations for Two-Phase Media*, Studies in Appl. Math. **50**, 133–166.

Goodman M.A. and Cowin S.C. (1972), *A Continuum Theory for Granular Materials*, Arch. Rational Mech. Anal. **44**, 249–266.

Kvasnica J. (1965), *Thermodynamics*, SNTL, Prague. (in Czech)

Truesdell C. (1984), *Rational Thermodynamics*, Springer–Verlag, New York.

Popis zrnitých materiálů pomocí průměrných hodnot

Ondřej Navrátil

V přírodě se velmi často vyskytují materiály, které lze v dobrém přiblížení považovat za materiály zrnité. V článku je popsána metoda středování, která popis zrnitého materiálu, mikroskopický popis, převádí na popis zrnitého materiálu pomocí rovnic mechaniky kontinua, makroskopický popis. Tato metoda využívá středování mikroskopických rovnic přes nějaký objem a časový interval. Střední hodnoty mechanických a termodynamických veličin definuji tak, abych získal rovnice mechaniky kontinua. Bohužel toto středování nedává žádné podmínky na konstitutivní vztahy pro zrnité materiály. Ty je při takovém středování nutné určit empiricky. Dále analyzuji pro zrnité materiály pojem absolutní teploty a entropie z hlediska obecných postulátů termodynamiky. Touto analýzou dospívám k závěru, že tyto veličiny nelze dobře pro zrnité materiály definovat.