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ON THERMODYNAMICS OF COMPLEX SYSTEMS

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О ТЕРМОДИНАМИКЕ СЛОЖНЫХ СИСТЕМ. Аркадий БЕРЕЗОВСКИЙ, Юри ЭНГЕЛЬБРЕХТ, Андраш СЕКЕРЕШ

Key words: thermodynamics, complex systems, thermoelasticity, internal variables.

Reported are the results presented at the workshop (May 3rd, 1993) held in the framework of the collaboration between the Department of Technical Mechanics, Budapest Technical University, and the Department of Mechanics, Institute of Cybernetics, Estonian Academy of Sciences. The month of intensive research was devoted to thermodynamics of complex systems.

Nonequilibrium thermodynamics has been formulated along two lines. The first is classical irreversible thermodynamics (CIT) and the second, rational thermodynamics (RT). A concise but transparent review of these theories is given by Lebon et al. [1]. However, both these theories have certain drawbacks including the paradox of infinite velocity. On the basis of earlier works by Cattaneo, Vernotte, Grad, and others, in the 1970s a new approach called extended irreversible thermodynamics (EIT) was proposed (see the references in [1]) that removed the paradox mentioned above and went beyond the hypothesis of local equilibrium. A little bit later hidden (internal) variable theory (HVT) was formed (see [2] and the references therein). Internal variables present some constraints in the sense of continuum mechanics and are not inertial, consequently their governing equations are mostly diffusion-reaction type. Despite the success of EIT and HVT, there are still many open problems related to complex and multiphase systems, nonlocality, etc. Not pretending to give an overview of these problems, we shall below discuss three aspects of thermodynamical theories, all related to basic mathematical models. The first deals with the consistency of heat conduction laws in thermoelasticity based on EIT and discusses the principles of equipresence and causality in the mathematical models. The second is related to basic concepts of thermodynamics of complex systems and, as a result, a modified equation of motion is derived. The third aspect is the role of internal variables in thermodynamics and their possible consequences on dynamics.

(i) Heat conduction problems. Conventional thermoelasticity (CTE) is based on CIT and RT and is widely used for solving practical problems, especially those thermal stresses (e. g. [3]). Later, on the basis of EIT, more sophisticated theories have been elaborated, like extended thermoelasticity (ETE) [4] or temperature-rate-dependent thermoelasticity (TRDTE) [5]. A detailed study shows that, bearing in mind the equipresence of all variables, their rates and gradients in governing equations, not all the variants of the heat conduction law are possible. Even more, consistent derivation leads to new terms in the heat conduction equation. As an example, one can derive on the basis of EIT

$$a\frac{\partial^2 T}{\partial x^2}=\frac{\partial T}{\partial t}+\tau_0\frac{\partial^2 T}{\partial t^2}+b\frac{\partial^2 T}{\partial x \partial t}, \tag{1}$$

where T is temperature, and a, b, τ_0 are constants [6]. The last term (mixed derivative) appears due to the temperature gradient in the expression of internal energy. A possible explanation of additional terms could be given in terms of microstructural properties of thermoelastic media, but more experimental and theoretical data are needed. One should point out that complexity of thermoelasticity is not based on the number of variables but on the different physical phenomena (mechanical and thermodynamical).

(ii) Thermodynamic formalism and continuum mehanics. The widely used concepts of conventional thermodynamics [7] are compared with those of a different approach, derived by Berezovsky and Rosenblum [8]. As it was noted by Kestin [7], "...this marriage between thermodynamics and continuum mechanics is neither simple nor straightforward". Therefore, considering a continuous body as a complex system containing the simple elements as constituents, the general principles for complex systems can be applied to the description of their behaviour. These principles, i. e. the principles of composition, interaction, invariance and duality are explicitly formulated and consistently used in [8]. As a result, the coexistence of various constituents in a continuous body leads to additional (thermodynamical) terms in equations of motion. For example, the homogeneous case yields

$$\varrho\frac{dw_i}{dt}=-\frac{\partial p}{\partial x_i}+\frac{\partial \sigma_{ij}}{\partial x_j}+\frac{\partial}{\partial x_i}\left[\left(\frac{\partial U}{\partial V}\right)_p\right], \tag{2}$$

where w_i are the components of the velocity vector (in x_i directions, respectively), σ_{ij} are the components of the stress tensor, ϱ is density, p is pressure, U is internal energy and V is volume.

In the heterogeneous case the thermodynamical term takes another form. It may happen that thermodynamical terms of different kinds become equal for the same constituent of a complex body. In such a singular situation the behaviour of a medium may be changed strongly. This may be a reason why organized structures appear in continuous media.

(iii) Internal variables and thermoelasticity. The mathematical models describing the dynamics of observable variables are based on hyperbolic models while internal variables are described either by kinetic or reaction-diffusion equations [2]. This leads to certain difficulties in deriving the evolution equations for coupled systems. On the other hand, internal variables obey the rules of continuum mechanics but need an additional potential, the so-called dissipation potential, to be introduced.

Examples of such potentials are given in [2,9]. Within the framework of CTE, temperature is also governed by the diffusion equation that formally leads to a similar situation. When the displacement U_i in CTE is treated as an observable and temperature T as an internal variable, then there exists a possibility of deriving an evolution equation for the gradient (or rate) of the displacement in the following form (1D case):

$$\frac{\partial u}{\partial \tau}+a_1 u\frac{\partial u}{\partial \xi}+a_2 u=0, \tag{3}$$

where $u\sim\partial U_1/\partial X_1\sim\partial U_1/\partial t$, $\tau\sim X_1$, $\xi\sim c_0 t-X_1$ and a_1, a_2 are coefficients. Such an evolution equation should be compared with the conventional Burgers equation derived on the basis of ETE [10].

A more detailed account of these problems can be found in [11].

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