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On thermodynamics, objectivity and the modeling of non-isothermal viscoelastic fluid behavior

H.S. da Costa Mattos [*]

Laboratório de Mecânica Teórica e Aplicada, Programa de Pós-Graduação em Engenharia Mecânica, Universidade Federal Fluminense, Rua Passo da Pátria 156, 24210-240, Niterói, RJ, Brazil

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ABSTRACT

The present paper is concerned with the modeling of non-isothermal viscoelastic fluid behavior. A general procedure, developed within the framework of thermodynamics of irreversible processes, is proposed to obtain constitutive relations that verify automatically the second law of thermodynamics and the principle of material objectivity. It is shown that the choice of the objective time derivative is important not only to assure a mathematically correct and physically realistic description of the viscoelastic behavior, but also to perform an adequate description of the thermomechanical coupling in the case of non-isothermal flows. Such a thermodynamic approach allows a rational identification of the terms responsible for the thermomechanical coupling in the heat equation, which is a first step to better understand their influence on the fluid behavior.

1. Introduction

Constitutive models for fluids are often classified as differential, rate and integral types [1–3]. To set up a general constitutive theory it is necessary to consider aspects of the first and second law of thermodynamics since heat transfer and dissipative behavior must be taken into account.

The constitutive theories in which the free energy is supposed to be a function of a set of independent variables [4], widely used in solid mechanics [5,6] but also for fluids [1–9], may provide practical tools for the modeling of non-Newtonian fluids, especially when it is necessary to account for the interference of the microstructure with the macrostructure. This is the case, for instance, of certain kinds of polymeric liquids in which the breakdown of connections between the structural units that characterize the internal (i.e. the submacroscopic) structure may induce a decrease in the resistance to flow [10,11].

In these theories, some variables are introduced to account for dissipative mechanisms. In a phenomenological approach, such additional variables are supposed to contain microstructural information, relevant for certain classes of materials. To each of these variables is associated one constitutive equation in such a way that a local version of the second law of thermodynamics must be satisfied. The study of viscoelastic fluids cannot be adequately performed without the analysis if a given set of objective constitutive equations is thermodynamically admissible or not.

Temperature plays an important role in complex flows of non-Newtonian fluids in many industrial applications, such as injection molding of polymers. Besides, an adequate modeling of the heat equation and a simple interpretation of the thermomechanical couplings is very important, mainly when dissipative mechanisms related to changes on the material structure or substructure must be taken into account.

This paper is concerned with the study of sufficient conditions for a thermodynamically consistent modeling of viscoelastic fluid behavior. A general procedure, developed within the framework of thermodynamics of irreversible

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[*] Tel.: +55 21 2629 5585; fax: +55 21 2629 5585.
E-mail address: heraldo@mec.uff.br.

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processes, is proposed to obtain constitutive relations that verify automatically the principle of material objectivity and a local version of the second law of thermodynamics. Such a procedure is similar to the one proposed in [12] by the author, but an even more general class of objective time derivatives is considered and the study is also focused on the analysis of the thermomechanical couplings that arise in the heat transfer equation. In the theory, the choice of a particular objective time derivative in rate type constitutive equations can be interpreted as a constitutive assumption. For each objective time derivative a particular measure of deformation is associated in order to assure that a local version of the second law of thermodynamics is automatically satisfied. The theory generalizes a great number of constitutive equations found in the literature allowing a simple modeling of important phenomena such as normal stress effects or the variability of viscosity with the rate of strain.

2. Preliminary definitions

Under suitable regularity assumptions it is possible to consider the following expressions as local versions of the first law (FLT) and second law of thermodynamics (SLT) [11,13]:

$$\text{FLT}: \rho\dot{e} = -\text{div}(\boldsymbol{q}) + \boldsymbol{T} : \boldsymbol{D} \tag{1}$$

$$\text{SLT}: d = \boldsymbol{T} : \boldsymbol{D} - \rho(\dot{\psi} + s\dot{\theta}) + \boldsymbol{q} \cdot \boldsymbol{g} \geq 0 \tag{2}$$

where $(\dot{\ })$ denotes the material time derivative of $()$; ρ is the mass density; $\boldsymbol{T}$ the Cauchy stress tensor; $\boldsymbol{D} = 1/2[\mathbf{grad}(\boldsymbol{v}) + \mathbf{grad}(\boldsymbol{v})^T]$ the deformation rate tensor; e the internal energy per unity mass, θ the absolute temperature; s the total entropy per unit mass; $\psi = (e - \theta s)$ the Helmholtz free energy per unit mass; $\boldsymbol{q}$ the heat flux vector and $\boldsymbol{g} = -\mathbf{grad}(\log\theta)$, $\log\theta$ standing for the logarithm of the absolute temperature. d is the rate of energy dissipation per unit volume.

The second law of thermodynamics makes a distinction between possible processes ($d \geq 0$) and impossible processes ($d < 0$). The possible processes may be reversible (the rate of energy dissipation d is always equal to zero) or not. This local version of the SLT does not exclude the possibility of unusual behaviors such as a decreasing temperature if heat is added to the medium. To exclude the possibility of such kind of unusual behavior, the present study is restricted to fluids that always satisfy a further restrictive constraint:

$$d_1 = \boldsymbol{T} : \boldsymbol{D} - \rho(\dot{\psi} + s\dot{\theta}) \geq 0 \tag{3}$$

$$d_2 = \boldsymbol{q} \cdot \boldsymbol{g} \geq 0. \tag{4}$$

Obviously, if the above relations are satisfied, then constraint (2) will also be satisfied. It is also simple to verify that (4) leads to the classical heat conduction inequality $-\boldsymbol{q}\cdot\mathbf{grad}(\theta) \geq 0$ since the absolute temperature θ is a positive quantity. This relation implies that heat flows in the direction of decreasing temperature when $\boldsymbol{q}$ is parallel to the temperature gradient. The quantity d_1, defined in Eq. (3), is usually called the intrinsic dissipation and the quantity d_2, defined in Eq. (4), the thermal dissipation.

3. Objective time derivatives

The material time derivative of an objective tensor quantity is not necessarily objective. Therefore, in order to assure objectivity, it is necessary to use some special kind of time derivative in rate type constitutive equations. A large number of definitions of objective time derivatives can be found in the literature (Jaumann, Truesdell, Cotter–Rivling, Gordon–Schowalter, etc. [11,14,15]). The choice of a particular derivative is important and can be interpreted as a constitutive assumption.

H1—The present study is restricted to the following family of derivatives:

$$\mathring{\mathbf{A}} = \dot{\mathbf{A}} + \mathbf{A}\boldsymbol{\Omega} - \boldsymbol{\Omega}\mathbf{A} - a(\mathbf{A}\boldsymbol{D} + \boldsymbol{D}\mathbf{A}) \tag{5}$$

where $\mathring{\mathbf{A}}$ is an objective time derivative of an arbitrary objective symmetric tensor $\mathbf{A}$. a is a scalar parameter such that $-1 \leq a \leq 1$ and $\boldsymbol{\Omega}$ is a time dependent second order tensor and differ with respect to the considered time derivative.

Expression (5) encompasses a great number of derivatives found in the literature, nevertheless, it is important to remark that, only if $a = 0$ in Eq. (5) it is possible to assure the following properties [16]

(i) The derivative of the unit tensor $\mathbf{1}$ vanishes

$$\mathring{\mathbf{1}} = \mathbf{0}. \tag{6}$$

(ii) Any objective rate of a symmetric tensor $\mathbf{A}$ should be symmetric

$$\mathring{\mathbf{A}} = (\mathring{\mathbf{A}})^T = (\mathring{\mathbf{A}^T}). \tag{7}$$