On compressible Korteweg fluid-like materials ☆

Martin Heida [a], Josef Málek [b,c,*]

[a] University of Heidelberg, Institute for Applied Mathematics, Im Neuenheimer Feld 294, 69120 Heidelberg, Germany
[b] Charles University, Faculty of Mathematics and Physics, Mathematical Institute, Sokolovská 83, 186 75 Prague 8, Czech Republic
[c] Institute of Thermomechanics, Academy of Sciences, Dolejškova 1402/5, 182 00 Prague 8, Czech Republic

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ABSTRACT

We provide a thermodynamic basis for compressible fluids of a Korteweg type that are characterized by the presence of the dyadic product of the density gradients $\nabla\varrho \otimes \nabla\varrho$ in the constitutive equation for the Cauchy stress. Our approach does not need to introduce any new or non-standard concepts such as multipolarity or interstitial working and is based on prescribing the constitutive equations for two scalars: the entropy and the entropy production. In comparison with the Navier–Stokes–Fourier fluids we suppose that the entropy is not only a function of the internal energy and the density but also of the density gradient. The entropy production takes the same form as for a Navier–Stokes–Fourier fluid. For a Navier–Stokes–Fourier fluid one can express the entropy production equivalently in terms of either thermodynamic affinities or thermodynamic fluxes. Following the ideas of K.R. Rajagopal concerning the systematic development of implicit constitutive theory and primary role of thermodynamic fluxes (such as force) that are *cause* of *effects* in thermodynamic affinities (such as deformation) in considered processes, we further proceed with a constitutive equation for entropy production expressed in terms of thermodynamic fluxes. The constitutive equation for the Cauchy stress is then obtained by maximizing the form of the rate of entropy production with respect to thermodynamic fluxes keeping as the constraint the equation expressing the fact that the entropy production is the scalar product of thermodynamic fluxes and thermodynamic affinities. We also look at how the form of the constitutive equation changes if the material in question is incompressible or if the processes take place at constant temperature. In addition, we provide several specific examples for the form of the internal energy and make the link to models proposed earlier. Starting with fully implicit constitutive equation for the entropy production, we also outline how the methodology presented here can be extended to non-Newtonian fluid models containing the Korteweg tensor in a straightforward manner.

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1. Introduction

In 1901, Korteweg published the paper [10] where he proposed to model phase transition phenomena in fluids by the stress tensor **T** depending on the gradient of the density ϱ and the gradient of the velocity $\boldsymbol{v}$ in the following manner

$$\mathbf{T} = (-p + \alpha_0|\nabla\varrho|^2 + \alpha_1\Delta\varrho)\mathbf{I} + \beta(\nabla\varrho \otimes \nabla\varrho) + 2\mu\mathbf{D}(\boldsymbol{v}) + \lambda(\mathrm{div}\,\boldsymbol{v})\mathbf{I}. \tag{1.1}$$

Here, p denotes the thermodynamic pressure being a function of ϱ, $\mathbf{D}(\boldsymbol{v})$ stands for the symmetric part of the velocity gradient and α_0, α_1, β, μ and λ are material moduli that may depend on ϱ as well.

One can split the complicated response (1.1) into the standard Navier–Stokes model for compressible fluids characterized by the constitutive equation

$$\mathbf{T}^{ns} = -p\mathbf{I} + 2\mu\mathbf{D}(\boldsymbol{v}) + \lambda(\mathrm{div}\,\boldsymbol{v})\mathbf{I}, \tag{1.2}$$

and the capillarity stress $\mathbf{T}^c$ of the form

$$\mathbf{T}^c = (\alpha_0|\nabla\varrho|^2 + \alpha_1\Delta\varrho)\mathbf{I} + \beta(\nabla\varrho \otimes \nabla\varrho). \tag{1.3}$$

The stress $\mathbf{T}^c$ was introduced to provide a smooth interface model as an alternative to the classical theory of sharp interfaces, which specifies a jump condition at the surface separating fluids possessing different densities.

It is also worth noting that the Cauchy stress formula (1.1) can be decomposed into the elastic and dissipative parts:

$$\mathbf{T}^{dis} = 2\mu\mathbf{D}(\boldsymbol{v}) + \lambda(\mathrm{div}\,\boldsymbol{v})\mathbf{I}, \tag{1.4}$$
$$\mathbf{T}^{elast} = (-p + \alpha_0|\nabla\varrho|^2 + \alpha_1\Delta\varrho)\mathbf{I} + \beta(\nabla\varrho \otimes \nabla\varrho). \tag{1.5}$$

Korteweg, see [10], derived a continuous model for fluids which can appear in their liquid and vapor phases. To this aim, he followed the idea of Van der Waals [20] who observed that the boundary between the two phases should not be a sharp interface but rather a thin transition zone of very steep density gradient. Based on this assumption Korteweg made some considerations on the possible interactions between the molecules in two neighbored infinitesimal representing volume elements and obtained an additional contribution to the stress tensor for the Navier–Stokes fluids which reads as

$$\mathbf{T}^c = \alpha|\nabla\varrho|^2\mathbf{I} + \beta\nabla\varrho \otimes \nabla\varrho - \gamma\Delta\varrho\mathbf{I} - \delta\nabla^{(2)}\varrho, \tag{1.6}$$

where especially the term $\beta\nabla\varrho \otimes \nabla\varrho$ is today generally known as Korteweg tensor.

Eq. (1.1) represents a very complicated relationship in comparison to (1.2) and there has been a constant, to our opinion not fully satisfactory, effort to find out whether or not the model (1.1) is consistent with the basic concepts of continuum thermodynamics, see Dunn and Serrin [6], Anderson et al. [1], Mehrabadi et al. [13]. In addition, one may be interested in various generalizations of (1.1) that would be capable to capture thermal effects, further non-Newtonian phenomena such as shear-thinning or stress relaxation, or on the other hand to get simplifications if the constraint of incompressibility of the material is applicable. This is certainly a non-trivial task in particular if one does it in an ad hoc manner.

Thus, one of the main points of this paper is to provide a thermodynamic well-sounded basis that would lead to (1.1) as a special case and that would be suitable for possible generalizations. There have been several approaches. Most of those based on the framework of continuum thermodynamics start with a general form for the Cauchy stress that is related explicitly to other quantities such as the velocity gradient, the density and their gradients (see for example [19]). This traditional approach usually results in models which have too many constants (or more generally material functions). The second law of thermodynamics is then used to provide restrictions on these coefficients. Due to apriori posed dependence of the stress tensor on the density gradient this method leads to some inconsistencies that were artificially overcome by introducing concepts such as the interstitial working, balance of self-equillibrated force system, multipolarity, see Dunn and Serrin [6], Anderson et al. [1], Cowin and Goodman [4], Mehrabadi et al. [13]. Our aim is to avoid any such questionable concepts.

The framework of the present approach is outlined by standard forms of the balance equation (mass, linear and angular momentum, energy) for a single continuum. Instead of making any assumption on the structure of the constitutive equation for the Cauchy stress *tensor* $\mathbf{T}$ we rather prescribe constitutive equations for two *scalars*: the entropy and the entropy production. In comparison with the Navier–Stokes–Fourier fluids we suppose that the entropy is not only a function of the internal energy and the density but also of the density gradient. The entropy production takes the same form as for the Navier–Stokes–Fourier fluid. While for Navier–Stokes–Fourier fluids one can express the entropy production equivalently in terms of either thermodynamic affinities or thermodynamic fluxes it seems essential for our study that we use the form expressed in terms of thermodynamic fluxes. We follow the ideas of K.R. Rajagopal concerning the systematic development of implicit constitutive theory (see [14,15]) and primary role of thermodynamic fluxes (such as force per unit area, heat flux) that cause changes in thermodynamic affinities (such as velocity and temperature gradients) in considered processes in a given material. The constitutive equations for the Cauchy stress and the heat flux are then obtained by maximizing the form of the entropy production with respect to thermodynamic fluxes keeping as the constraint the equation expressing the fact that the rate of entropy production is the scalar product of thermodynamic fluxes and thermodynamic affinities.

The approach presented here carries on several recent studies connected with ideas of K.R. Rajagopal. The contributions which have a very strong impact on the appearance of this work are the following: (1) The paper by Rajagopal and Srinivasa [17] where a general robust framework to constitutive theory in the area of continuum thermodynamics is described. They also present in detail the concept of natural configuration and the role/meaning of a principle of maximization of the entropy production in the systematic derivation of constitutive relations. (2) The paper by Rajagopal and Srinivasa [18] where implicit constitutive theory is combined with the principle of maximization of entropy production in which maximization is taken with respect to thermodynamic fluxes for the first time. (3) The paper [11] where the authors were successful in