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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 that does not need to introduce any new or non-standard concepts such as for example multipolarity or interstitial working 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 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 the 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.

To Professor K. R. Rajagopal on the occasion of his 60th birthday

1. INTRODUCTION

In 1901, Korteweg publishes the paper [7] where he proposes to model phase transition phenomena in fluids by the stress tensor $\mathbf{T}$ depending on the gradient of the density ϱ and the gradient of the velocity $\boldsymbol{v}$ in the following manner

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

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 fluid characterized by the constitutive equation

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

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

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

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

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

$$(1.4) \qquad\qquad \mathbf{T}^{dis} = 2\mu\mathbf{D}(\boldsymbol{v}) + \lambda(\operatorname{div}\boldsymbol{v})\mathbf{I}$$

$$(1.5) \qquad\qquad \mathbf{T}^{elast} = (-p + \alpha_0|\nabla\varrho|^2 + \alpha_1\Delta\varrho)\mathbf{I} + \beta(\nabla\varrho\otimes\nabla\varrho)\,.$$

Korteweg, see [7], derived a continuous model for fluids which can appear in its liquid and vapor phases. To this aim, he followed the idea of van der Waals [15] 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 obtain an additional contribution to the stress tensor for the the Navier-Stokes fluids which reads as

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

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

Equation (1.1) represents a very complicated relationship in comparison to (1.2) and there has been a constant effort to find out whether or not the model (1.1) is consistent with the basic concepts of continuum thermodynamics, see Dunn and Serrin [5], Anderson et al. [1], Mehrabadi et al. [10]. 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 see simplifications if the constraint of incompressibility of the material is applicable[1]. This is certainly a nontrivial task in particular if one does it in an adhoc 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 starts with a general form for the Cauchy stress that is related explicitly to other quantities as those such as the velocity gradient, the density and their gradients, see for example [14]. This traditional approach usually results at the model that 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

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[1]We are also interested in observing if the Cauchy stress being a sum of the original Korteweg form (1.6) and the Navier-Stokes form (1.2) is themodynamicly consistent.

density gradient this method leads to some inconsistencies that were artificially overcome by introducing the concepts such as the interstitial working or multipolarity, see Dunn and Serrin [5], Anderson et al. [1], Mehrabadi et al. [10]. Our aim is to avoid any such questionable concepts.

The framework 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 a Navier-Stokes-Fourier fluids one can express the entropy production equivalently in the 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 developmnet of implicit constitutive theory 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 that has very strong impact on the appearance of this work are the following: (1) the paper by Rajagopal and Srinivasa [12] where a general framework to constitutive theory in the area of continuum thermodynamics is described and the concept of natural configuration and the role/meaning of a principle of maximization of the entropy production in systematic derivation of the constitutive relations are presented in detail, (2) the paper by Rajagopal and Srinivasa [13] where implicit constitutive theory is combined with the principle of maximization of entropy production in which maximization is, for the first time, taken with respect to thermodynamic fluxes, (3) the paper [8] where the authors were successful in deriving an hierarchy of models for *incompressible* materials of Korteweg-type and (4) the paper [9] where thermodynamics for compressible non-Newtonian fluids given through implicit constitutive relations is developed.

The scheme of the paper is the following. In the next section, we introduce our framework and make its link to classical fluid thermodynamics described by the Navier-Stokes-Fourier fluids. Then we derive constitutive equations involving the Cauchy stress and the heat flux starting with the constitutive equation for two scalars: the entropy depending on the internal energy, the density and its gradient, and the entropy production expressed in thermodynamic fluxes being of the same form as for the Navier-Stokes-Fourier fluid. Then we concentrate on specific forms of the constitutive equation for the internal energy (which is equivalent to the constitutive equation for the entropy) and make links to earlier engineering and mathematical studies. In the concluding section we discuss the possible extensions (to non-Newtonian fluids in particular).

2. Balance equations. Second law of thermodynamics. Compressible Navier-Stokes-Fourier fluid.

2.1. **Balance equations.** At the continuum level, motions of fluids are usually described in terms of the density ϱ, the velocity field $\boldsymbol{v} = (v_1, v_2, v_3)$, the internal energy e, the Cauchy stress

$\mathbf{T} = \{T_{ij}\}_{i,j=1}^3$ and the heat flux $\boldsymbol{q} = (q_1, q_2, q_3)$ through the system of equations that are a consequence of the balance of mass, balance of linear and angular momentum, and balance of energy applied to each sub-volume of the material, that lead to local forms for these balance laws in the form

$$
\begin{aligned}
\dot{\varrho} &= -\varrho \operatorname{div} \boldsymbol{v} \,,
\end{aligned}
$$

(2.1)
$$
\varrho \dot{\boldsymbol{v}} = \operatorname{div} \mathbf{T} + \varrho \boldsymbol{f} \,, \qquad \mathbf{T} = \mathbf{T}^T \,,
$$

$$
\varrho \dot{E} = \operatorname{div}(\mathbf{T}\boldsymbol{v} - \boldsymbol{q}) + \varrho r + \varrho \boldsymbol{f} \cdot \boldsymbol{v} \,,
$$

where $E = \frac{1}{2}|\boldsymbol{v}|^2 + e$ (the total energy) is the sum of specific kinetic energy $\frac{1}{2}|\boldsymbol{v}|^2$ and specific internal energy e, $\boldsymbol{f}$ represents the specific body forces (such as gravity) and r stands for the specific production of energy (radiation, for example).

For any scalar quantity z, the symbol $\dot{z}$ denotes the material derivative of z that can be expressed as

$$
\dot{z} = z_{,t} + \nabla z \cdot \boldsymbol{v} = \frac{\partial z}{\partial t} + \sum_{k=1}^3 \frac{\partial z}{\partial x_k} v_k \,.
$$

In order to avoid misunderstanding, we sometimes prefer to use $\dot{\overline{z}}$ instead of $\dot{z}$.

For further purpose, it is worth observing that $(2.1)_1$ implies that

(2.2)
$$
\dot{\overline{\nabla \varrho}} = -[\nabla \boldsymbol{v}] \nabla \varrho - (\operatorname{div} \boldsymbol{v}) \nabla \varrho - \varrho \nabla \operatorname{div} \boldsymbol{v} \,.
$$

2.2. **Assumption of maximization of entropy production.** Following Callen [3], we assume the existence of specific entropy η as a differentiable function of the internal energy e and other state variables $\boldsymbol{y} = (y_1, \ldots, y_M)$, i.e., $\eta = \tilde{\eta}(e, \boldsymbol{y})$ such that $\tilde{\eta}$ is increasing with respect to e. The inverse function theorem then implies that

(2.3)
$$
e = \tilde{e}(\eta, \boldsymbol{y}) \,.
$$

Setting $\theta := \dfrac{\partial \tilde{e}}{\partial \eta}$, which is always positive, differentiation of (2.3) leads to the equation

(2.4)
$$
\theta \dot{\eta} = \dot{e} - \frac{\partial \tilde{\eta}}{\partial \boldsymbol{y}} \cdot \dot{\overline{\boldsymbol{y}}} = \dot{E} - \boldsymbol{v} \cdot \dot{\boldsymbol{v}} - \frac{\partial \tilde{\eta}}{\partial \boldsymbol{y}} \cdot \dot{\overline{\boldsymbol{y}}} \,.
$$

Inserting the balance equations (2.1) into (2.4), using the equation for $\dot{\overline{\boldsymbol{y}}}$ that however come from the specific choice of state variables $\boldsymbol{y}$ (it means from *the constitutive equation for the entropy* or equivalently from (2.3)), we end-up with the equation for the evolution of specific entropy η written in the form of balance equation

(2.5)
$$
\varrho \dot{\eta} + \operatorname{div}\left(\frac{\boldsymbol{h}}{\theta}\right) = \frac{\xi}{\theta} \,,
$$

where $\boldsymbol{h}/\theta$ stands for the entropy flux and ξ is the entropy production that has the form

(2.6)
$$
\xi = \sum_\alpha J_\alpha A_\alpha \,.
$$

In (2.6), J_α represents thermodynamic fluxes and A_α thermodynamic affinities.

The second law of thermodynamics states that the entropy production has to be nonnegative. In the approach developed by Rajagopal and Srinivasa in the late nineties (see [12] for a careful and detailed discussion of several relevant issues and earlier studies) one prescribes a constitutive

form for the entropy production ξ that is apriori *nonnegative* and thus the second law of thermodynamics is automatically fulfilled. To give such a constitutive relation is not an easy task since it requires to know what are the relevant dissipative mechanisms that take place in considered processes in considered materials. In general case, we assume the constitutive equation for ξ of the form

$$(2.7) \qquad \xi = \tilde{\xi}(J_\alpha, A_\alpha) \geq 0 \,.$$

Let us recall that we have prescribed (assumed), up to this point, two constitutive relationships, namely (2.3) and (2.6), for two scalar quntities: the entropy η (or the internal energy e) and the entropy production ξ. Constitutive equations that relates thermodynamic affinities to thermodynamic fluxes and state variables are then determined by applying *the assumption (principle) of maximization of entropy production*. This is a constrained maximization method, see [12] for details, in which the constitutive equations are obtained at maximal value of $\tilde{\xi}$ of the form (2.7) whereas one requires that (2.6) holds as the constraint and one maximizes $\tilde{\xi}$ with respect to J_α (thermodynamic fluxes). Said differently, if we assume that $\tilde{\xi}$ is a nonnegative differentiable function of variables J_α and A_α, which is in addition convex with respect to J_α, then the inquired constitutive equations coincides with necessary conditions of the constrained maximization problem

$$(2.8) \qquad \max_{J_\alpha} \tilde{\xi}(J_\alpha, A_\alpha) \quad \text{provided that (2.6) holds} \,.$$

Clearly, these necessary conditions then read

$$(2.9) \qquad \frac{\partial \tilde{\xi}}{\partial J_\alpha} + \lambda \left(\frac{\partial \tilde{\xi}}{\partial J_\alpha} - A_\alpha \right) = 0 \quad \Longleftrightarrow \quad A_\alpha = \frac{1+\lambda}{\lambda} \frac{\partial \tilde{\xi}}{\partial J_\alpha} \,.$$

In this study, we consider a very simpler form for $\tilde{\xi}$, namely

$$(2.10) \qquad \tilde{\xi}(J_\alpha) = \sum_\alpha \frac{1}{\gamma_\alpha} |J_\alpha|^2 \,,$$

where γ_α are positive constants or functions of state variables. Instead of arguing on a general level why we make this particular choice of $\tilde{\xi}$, we discuss advantages of this form below for the case of classical Navier-Stokes-Fourier fluid.

It follows from (2.7), (2.9) and (2.10) that $\frac{1+\lambda}{\lambda} = \frac{1}{2}$ and

$$(2.11) \qquad A_\alpha = \frac{1}{\gamma_\alpha} J_\alpha \quad \Longleftrightarrow \quad J_\alpha = \gamma_\alpha A_\alpha \,.$$

We conclude this part by summarizing characteristic features of the approach. In order to apply the above outlined framework we need to

- specify the state variable $\boldsymbol{y}$ and thus identify the constitutive equation (2.3),
- compute the form of the entropy flux $\boldsymbol{h}$ and the entropy production ξ in (2.5) and thus identify thermodynamic fluxes J_α and corresponding thermodynamic affinities A_α,
- write down the constitutive equation (2.11) being however aware of a particular form (2.10) we used in deriving (2.11).

In the next subsection, we consider a Navier-Stokes-Fourier fluid ($\boldsymbol{y}$ contains merely one component ϱ and $e = \tilde{e}(\eta, \varrho)$). The reason why we recall this basic fluid model is twofold. First, we wish to motivate as clear as possible the particular form of the constitutive equation for the

entropy production that we will use in Section 3. Second, we illustrate the efficacy of the above framework.

In Section 3, we apply the above framework assuming that $\boldsymbol{y} = (\varrho, \nabla \varrho)$ and $e = \tilde{e}(\eta, \varrho, \nabla \varrho)$ and taking the same form for the entropy production as in the case of a Navier-Stokes-Fourier fluid, and obtain the constitutive equations involving Korteweg stress.

2.3. **Classical compressible Navier-Stokes-Fourier fluid.** We start with the classical definition of a compressible Navier-Stokes-Fourier fluid characterized by the constitutive equations

$$(2.12) \qquad \mathsf{T} = -p(\eta, \varrho)\mathsf{I} + 2\mu(\eta, \varrho)\mathsf{D}^d + \frac{2\mu(\eta, \varrho) + 3\lambda(\eta, \varrho)}{3}(\operatorname{div} \boldsymbol{v})\mathsf{I},$$
$$\boldsymbol{q} = k(\eta, \varrho)\nabla\theta \quad \text{and } r = 0,$$

where p is the thermodynamic pressure and $\mathsf{D}^d = \mathsf{D} - \frac{1}{3}(\operatorname{tr}\mathsf{D})\mathsf{I} = \mathsf{D} - \frac{1}{3}(\operatorname{div} \boldsymbol{v})\mathsf{I}$ is deviatoric part of D.

Setting

$$(2.13) \qquad m := \frac{1}{3}\operatorname{tr}\mathsf{T} \quad \text{and} \quad \mathsf{T}^d := \mathsf{T} - m\mathsf{I},$$

we observe that it is possible to rewrite the relationships (2.12) in the following forms

$$m + p(\eta, \varrho) = \frac{2\mu(\eta,\varrho)+3\lambda(\eta,\varrho)}{3}(\operatorname{div} \boldsymbol{v}) \quad \Longleftrightarrow \quad \operatorname{div} \boldsymbol{v} = \frac{3}{2\mu(\eta,\varrho)+3\lambda(\eta,\varrho)}(m + p(\eta, \varrho)),$$

$$(2.14) \qquad \mathsf{T}^d = 2\mu(\eta, \varrho)\mathsf{D}^d \quad \Longleftrightarrow \quad \mathsf{D}^d = \frac{1}{2\mu(\eta, \varrho)}\mathsf{T}^d,$$

$$\boldsymbol{q} = -k(\eta, \varrho)\nabla\theta \quad \Longleftrightarrow \quad \nabla\theta = -\frac{1}{k(\eta, \varrho)}\boldsymbol{q}.$$

While the equations that are written first in (2.14) represent the usual forms in which the constitutive equations for the Navier-Stokes-Fourir fluid are formulated, the equations that are written as second in (2.14) reflect better the fact that changes in $m + p(\varrho)$, T^d and $\boldsymbol{q}$ initiate the changes in $\operatorname{div} \boldsymbol{v}$, D^d and $\nabla\theta$, respectively.

In order to identify the quantities $\boldsymbol{h}$ and ξ in the equation (2.5) we recall that $e = \tilde{e}(\eta, \varrho)$ and then (2.4) takes the form

$$(2.15) \qquad \varrho\theta\dot{\eta} = \varrho\dot{E} - \boldsymbol{v} \cdot \varrho\dot{\boldsymbol{v}} - \varrho\frac{\partial\tilde{\eta}}{\partial\varrho}\dot{\varrho}.$$

Inserting the balance equations (2.1) into (2.15) we conclude, see [9] for details, that $\boldsymbol{h} = \boldsymbol{q}$ and

$$(2.16) \qquad \xi = \mathsf{T}^d \cdot \mathsf{D}^d + (m + p(\eta, \varrho))\operatorname{div} \boldsymbol{v} + (-\boldsymbol{q}) \cdot \frac{\nabla\theta}{\theta},$$

where we set

$$p(\eta, \varrho) = \varrho^2\frac{\partial\tilde{\eta}}{\partial\varrho}(\eta, \varrho).$$

At this point, we insert the constitutive equations (2.14) into (2.16) following the aim to get some insight concerning the structure of ξ. Note that there two conceptually different possibilities how to do it: either to use the forms written in the first column of (2.14) or use the formulas in the second column. Inserting the left column of (2.14) into (3.7) we obtain the traditional form for the entropy production, namely $(\kappa(\dots) := k(\dots)/\theta)$

$$(2.17) \qquad \xi = 2\mu(\eta, \varrho)|\mathsf{D}^d|^2 + \frac{2\mu(\eta,\varrho)+3\lambda(\eta,\varrho)}{3}(\operatorname{div} \boldsymbol{v})^2 + \kappa(\eta, \varrho)|\nabla\theta|^2,$$

while inserting the relations at the right column of (2.14) into (3.7) we conlude that

$$(2.18) \qquad \xi = \frac{1}{2\mu(\eta,\varrho)}|\mathbf{T}^d|^2 + \frac{3}{2\mu(\eta,\varrho)+3\lambda(\eta,\varrho)}(m + p(\eta,\varrho))^2 + \frac{1}{\kappa(\eta,\varrho)}|\boldsymbol{q}|^2 \,.$$

As addressed in [9], the form (2.18) provides better inside to understanding when a given material does not dissipate any energy (i.e. produces no entropy). A Navier-Stokes-Fourier fluid does not produce any entropy if it is in a process in which neither volume changes nor any isochoric dissipative processes as shear nor any heat flux generation take place. If this happens, then, in such a process, a fluid in consideration behaves as a compressible Euler fluid. On contrary, the traditional form (2.17) usually leads to a conclusion that the fluid does not produce any entropy if the material moduli (shear viscosity μ, bulk viscosity $\frac{2\mu(\eta,\varrho)+3\lambda(\eta,\varrho)}{3}$ and heat conductivity κ) are zero. Note that the form (2.18) is meaningful only if the material coefficients are positive. Also, a popular formulation of the Stokes hypothesis says that the bulk viscosity is zero, however, its physical formulation "minus mean normal stress m equals the thermodynamic pressure p" is not only better readable from (2.18) but (2.18) also clarifies under what conditions Stokes' hypothesis is acceptable; it is when there is no dissipation of energy associated with the volume changes.

We finallly perform an "inverse" operation: assuming the constitutive relationships for the *scalar* quantity ξ of the form (2.18), we aim to obtain the constitutive relationship for $\mathbf{T}$. As explained in previous subsection, this is achieved by maximizing ξ with respect to m and the components of $\mathbf{T}^d$ and $\boldsymbol{q}$, and also requiring that the identity (2.16) holds as a constraint. It follows from a general scheme described in Subsct. 2.2 that this maximization process leads directly to the relations listed at the right column of (2.14).

It is worth mentioning that starting with the form (2.17) where ξ is expressed in terms of thermodynamic affinities the analogous maximization process results at the constitutive equations written at the left column of (2.14). Thus, despite the fact that there are several arguments supporting the preference of (2.18) to (2.17), in the case of the Bavier-Stokes-Fourier fluid, it does not matter if we use (2.17) and maximize with respect to div $\boldsymbol{v}$, $\mathbf{D}^d$ and $\nabla\theta$ or if we use (2.18) and maximize with respect to $m + p$, $\mathbf{T}^d$ and $\boldsymbol{q}$; the both approaches lead to the same answer. We will however see in the next section that it seems important for derivation of constitutive equations involving Korteweg stress to consider constitutive equation for the production of entropy of the form (2.18).

3. Heat-conducting fluids of Korteweg-type. General form

We aim to derive the constitutive equations involving the Cauchy stress and the heat flux for compressible (and incompressible) heat-conducting fluid-like materials so that Korteweg tensor is included into the constitutive equation for the Cauchy stress. We procceed in the way described on a general level in Subsection 2.2.

We first make a choice of state variables and assume that the specific entropy is increasing differentiable function of the internal energy, the density and the density gradient and as a consequence of it we have

$$(3.1) \qquad e = \tilde{e}(\eta, \varrho, \nabla\varrho) \quad \text{and} \quad \theta := \frac{\partial\tilde{e}}{\partial\eta} > 0 \,.$$

Applying the material time derivative to (3.1), we obtain

$$\varrho\dot{e} = \varrho\frac{\partial\tilde{e}}{\partial\eta}\dot{\eta} + \varrho\frac{\partial\tilde{e}}{\partial\varrho}\dot{\varrho} + \varrho\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\cdot\dot{\overline{\nabla\varrho}} \,,$$

and thus, using all the equations listed in (2.1), (2.2) and $(3.1)_2$, we conclude that

$$\varrho\theta\dot{\eta} = \left(\mathbf{T} + \varrho\left(\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\otimes\nabla\varrho\right)\right)\cdot\nabla\boldsymbol{v} + \varrho^2\frac{\partial\tilde{e}}{\partial\varrho}\operatorname{div}\boldsymbol{v} + \left(\varrho\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\cdot\nabla\varrho\right)\operatorname{div}\boldsymbol{v}$$

(3.2)

$$- \operatorname{div}\boldsymbol{q} + \varrho r + \varrho^2\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\cdot\nabla\operatorname{div}\boldsymbol{v}\,,$$

which we rewrite as

$$\varrho\theta\dot{\eta} = \left(\mathbf{T} + \varrho\left(\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\otimes\nabla\varrho\right)\right)\cdot\nabla\boldsymbol{v} + \left(\varrho^2\frac{\partial\tilde{e}}{\partial\varrho} + \varrho\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\cdot\nabla\varrho - \operatorname{div}\left(\varrho^2\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\right)\right)\operatorname{div}\boldsymbol{v}$$

(3.3)

$$- \operatorname{div}\left(\boldsymbol{q} - \varrho^2\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\operatorname{div}\boldsymbol{v}\right) + \varrho r\,.$$

Referring to the notation $\mathbf{T}^d$, $\mathbf{D}^d$ and m defined above and setting

$$p = p(\eta,\varrho,\nabla\varrho) = \varrho^2\frac{\partial\tilde{e}}{\partial\varrho} \qquad\qquad\text{(generalized thermodynamic pressure)}$$

$$P = p + \frac{4}{3}\varrho\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\cdot\nabla\varrho - \operatorname{div}\left(\varrho^2\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\right)\,,$$

(3.4) $$\tilde{P} = P + \varrho^2\nabla\theta\cdot\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\,,$$

$$\boldsymbol{h} = \boldsymbol{q} - \varrho^2(\operatorname{div}\boldsymbol{v})\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\,,$$

$$\mathbf{T}^{dis} = \mathbf{T}^d + \varrho\left(\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\otimes\nabla\varrho - \frac{1}{3}\left(\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\cdot\nabla\varrho\right)\mathbf{I}\right)\,,$$

we shorten the equation (3.3) into the form

(3.5) $$\varrho\theta\dot{\eta} = \mathbf{T}^{dis}\cdot(\nabla\boldsymbol{v})^d + (P+m)\operatorname{div}\boldsymbol{v} - \operatorname{div}\boldsymbol{h} + \varrho r\,.$$

Consequently

$$\varrho\dot{\eta} + \operatorname{div}\left(\frac{\boldsymbol{h}}{\theta}\right) = \frac{1}{\theta}\left[\mathbf{T}^{dis}\cdot(\nabla\boldsymbol{v})^d + (P+m)\operatorname{div}\boldsymbol{v} - \left(\frac{\boldsymbol{h}}{\theta}\right)\cdot\nabla\theta + \varrho r\right]$$

(3.6)

$$= \frac{1}{\theta}\left[\mathbf{T}^{dis}\cdot(\nabla\boldsymbol{v})^d + \left(m + P + \varrho^2\nabla\theta\cdot\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\right)\operatorname{div}\boldsymbol{v} - \left(\frac{\boldsymbol{q}}{\theta}\right)\cdot\nabla\theta + \varrho r\right]$$

$$= \frac{1}{\theta}\left[\mathbf{T}^{dis}\cdot(\nabla\boldsymbol{v})^d + \left(m + \tilde{P}\right)\operatorname{div}\boldsymbol{v} - \left(\frac{\boldsymbol{q}}{\theta}\right)\cdot\nabla\theta + \varrho r\right]\,,$$

which is of the form (2.5). The terms that appear on the right-hand side of (3.6) represent the entropy producing mechanisms associated with different physical changes that take place in the body. It is worth noticing that the production of entropy ξ is indeed of the form (2.6) and can be written in the form of scalar product of the fourteen-dimensional vector of thermodynamic fluxes $(\mathbf{T}^d, m + \tilde{P}, \boldsymbol{q}/\theta, r)$ and the vector of thermodynamic affinities $(\mathbf{D}^d, \operatorname{div}\boldsymbol{v}, \nabla\theta, \varrho)$.

We set $r = 0$ in what follows. If the tensors $\mathbf{T}$ and $\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\otimes\nabla\varrho$ are symmetric then $\mathbf{T}^{dis}$ is symmetric as well. Note that it follows from (3.4) that $\mathbf{T}^{dis}$ is traceless. Under such circumstances, the production of entropy, i.e., θ multiplier of the right hand side of (3.6), simplifies to

(3.7) $$\xi = \mathbf{T}^{dis}\cdot\mathbf{D}^d + (m + \tilde{P})\operatorname{div}\boldsymbol{v} + (-\boldsymbol{q})\cdot\frac{\nabla\theta}{\theta}\,.$$

In what follows, we shall consider Newtonian-like fluids in which heat is conducted following the Fourier law. Thus, in accordance with (2.10) and (2.18), we assume that

(3.8) $\quad \xi = \tilde{\xi}(\varrho, \theta, \mathbf{T}^{dis}, m, \boldsymbol{q}) := \frac{1}{2\mu(\varrho,\theta)}|\mathbf{T}^{dis}|^2 + \frac{3}{2\mu(\varrho,\theta)+3\lambda(\varrho,\theta)}(m + \tilde{P}(\varrho, \nabla\varrho, \theta, \nabla\theta))^2 + \frac{1}{\kappa(\varrho,\theta)}|\boldsymbol{q}|^2 \,,$

where μ, $2\mu + 3\lambda$ and κ are positive.

Referring to the principle of maximizing the entropy production described on a general level in Subsection 2.2 and applying it to our specific setting given by (3.6) and (3.8), we conclude from (2.11) that

$$\mathbf{D}^d = \frac{1}{2\mu(\ldots)}\mathbf{T}^{dis}\,,$$

(3.9) $$\operatorname{div}\boldsymbol{v} = \frac{3}{2\mu(\ldots)+3\lambda(\ldots)}(m + \tilde{P}(\ldots))\,,$$

$$\nabla\theta = \frac{\theta}{\kappa(\ldots)}\boldsymbol{q}\,.$$

or in compact form

$$\mathbf{T}^{dis} = 2\mu(\ldots)\mathbf{D}^d\,,$$

(3.10) $$m = \frac{2\mu(\ldots)+3\lambda(\ldots)}{3}\operatorname{div}\boldsymbol{v} - \tilde{P}(\ldots))\,,$$

$$\boldsymbol{q} = k(\ldots)\nabla\theta\,. \qquad (k := \kappa/\theta)$$

Upon inserting (3.10) into (3.4) we finally obtain

(3.11)
$$\begin{aligned}
\mathbf{T} = \mathbf{T}^d + m\mathbf{I} &= \mathbf{T}^{dis} - \varrho\left(\frac{\partial\tilde{e}}{\partial\boldsymbol{z}} \otimes \nabla\varrho - \frac{1}{3}\left(\frac{\partial\tilde{e}}{\partial\boldsymbol{z}} \cdot \nabla\varrho\right)\mathbf{I}\right) + m\mathbf{I} \\
&= 2\mu\mathbf{D}^d - \varrho\left(\frac{\partial\tilde{e}}{\partial\boldsymbol{z}} \otimes \nabla\varrho - \frac{1}{3}\left(\frac{\partial\tilde{e}}{\partial\boldsymbol{z}} \cdot \nabla\varrho\right)\mathbf{I}\right) + \frac{2\mu(\ldots)+3\lambda(\ldots)}{3}(\operatorname{div}\boldsymbol{v})\mathbf{I} \\
&\quad - \varrho^2\left(\frac{\partial\tilde{e}}{\partial\boldsymbol{z}} \cdot \nabla\theta\right)\mathbf{I} - p\mathbf{I} - \frac{4}{3}\varrho\left(\frac{\partial\tilde{e}}{\partial\boldsymbol{z}} \cdot \nabla\varrho\right)\mathbf{I} + \operatorname{div}\left(\varrho^2\frac{\partial\tilde{e}}{\partial\boldsymbol{z}}\right)\mathbf{I} \\
&= 2\mu\mathbf{D} + \lambda(\operatorname{div}\boldsymbol{v})\mathbf{I} - \varrho\frac{\partial\tilde{e}}{\partial\boldsymbol{z}} \otimes \nabla\varrho + \varrho\operatorname{div}(\varrho\frac{\partial e}{\partial\boldsymbol{z}})\mathbf{I} - p\mathbf{I} - \varrho^2\left(\frac{\partial\tilde{e}}{\partial\boldsymbol{z}} \cdot \nabla\theta\right)\mathbf{I}\,.
\end{aligned}$$

The last formula expresses the constitutive equations characterizing a class of Navier-Stokes-Fourier-Korteweg fluids that is consistent with basic principles of continuum thermodynamics. It is interesting to notice that we "avoid" difficulties that appeared at earlier studies since (i) we do not assume apriori that the entropy flux equals $\boldsymbol{q}/\theta$ and (ii) following Rajagopal [11] (see also [13], [9]) we express the entropy production in terms of thermodynamic fluxes and not, as it is traditionally done, in thermodynamic affinities.

Before focusing on specific choice of the constitutive equation for e, we will look at the consequences of the above approach if we consider materials that are incompressible.

3.1. Incompressible heat-conducting fluids of Korteweg-type.
If the fluid is incompressible and inhomogeneous, i.e. $\operatorname{div}\boldsymbol{v} = 0$, then (3.7) simplifies to

(3.12) $$\xi = \mathbf{T}^{dis} \cdot \mathbf{D}^d + (-\boldsymbol{q}) \cdot \frac{\nabla\theta}{\theta}\,.$$

It then also follows from the framework described above that the constitutive equation for ξ cannot depend on m and m cannot be determined constitutivly.

Thus, assuming, instead of (3.7), that the constitutive equation for ξ takes the form

$$(3.13) \qquad \xi = \tilde{\xi}(\varrho, \theta, \mathbf{T}^{dis}, \boldsymbol{q}) := \frac{1}{2\mu(\varrho, \theta)}|\mathbf{T}^{dis}|^2 + \frac{1}{\kappa(\varrho, \theta)}|\boldsymbol{q}|^2 \,,$$

we observe that the system of governing equations

$$(3.14) \qquad \operatorname{div} \boldsymbol{v} = 0\,, \quad \dot{\varrho} = 0\,, \quad \varrho\dot{\boldsymbol{v}} = \operatorname{div}\mathbf{T} + \varrho\boldsymbol{f}\,, \quad \varrho\dot{E} = \operatorname{div}(\mathbf{T}\boldsymbol{v} - \boldsymbol{q}) + \varrho\boldsymbol{f} \cdot \boldsymbol{v}$$

is completed by the constitutive relations

$$(3.15) \qquad \begin{aligned} \mathbf{T} &= m\mathbf{I} + 2\mu(\dots)\mathbf{D}(\boldsymbol{v}) - \varrho\frac{\partial\tilde{e}}{\partial\boldsymbol{z}} \otimes \nabla\varrho\,, \\ \boldsymbol{q} &= k(\dots)\nabla\theta\,. \end{aligned}$$

These constitutive equations coincides with those derived in [8] where however the constitutive equation for the entropy production is expressed in terms of thermodynamic affinities. As shown, for incompressible fluids it does not matter what kind of form is used to obtain incompressible Navier-Stokes-Fourier-Korteweg fluid models.

4. Examples of Navier-Stokes-Korteweg fluids

In this section we discuss various specific forms of Korteweg stress that are consequences of different structural form of the constitutive equation for $\tilde{e}$ being a function of η, ϱ and $\nabla\varrho$. We will give some examples for the stress tensor associated with capillary effects. For simplicity, we only consider isothermal processes, i.e. $\boldsymbol{q} = \boldsymbol{0}$ and consequently $\nabla\theta = \boldsymbol{0}$.

We start from the general form of the stress tensor given in equation (3.11)

$$\mathbf{T} = 2\mu(\dots)\mathbf{D} + \lambda(\dots)(\operatorname{div}\boldsymbol{v})\mathbf{I} - \varrho\frac{\partial\tilde{e}}{\partial\boldsymbol{z}} \otimes \nabla\varrho + \varrho\operatorname{div}(\varrho\frac{\partial\tilde{e}}{\partial\boldsymbol{z}})\mathbf{I} - p\mathbf{I} - \varrho^2\frac{\partial\tilde{e}}{\partial\boldsymbol{z}} \cdot \nabla\theta\mathbf{I}\,.$$

We denote by $\tilde{\mathbf{T}}^c$ the sum of all terms which are not due to viscous effects, i.e.

$$\tilde{\mathbf{T}}^c := -\varrho\frac{\partial\tilde{e}}{\partial\boldsymbol{z}} \otimes \nabla\varrho + \varrho\operatorname{div}(\varrho\frac{\partial\tilde{e}}{\partial\boldsymbol{z}})\mathbf{I} - p\mathbf{I} - \varrho^2\frac{\partial\tilde{e}}{\partial\boldsymbol{z}} \cdot \nabla\theta\mathbf{I}\,.$$

We furthermore assume that the internal energy $\tilde{e}$ is given as a sum of pure volumetric energy e_0 depending only on ϱ and η and a term of capillary energy $\hat{e}$ depending on ϱ and $\nabla\varrho$

$$(4.1) \qquad \tilde{e} = e_0(\eta, \varrho) + \hat{e}(\varrho, \nabla\varrho)\,.$$

This implies that the generalized thermodynamic pressure p also splits up into

$$p = p_0 + p_c \quad \text{with } p_0 := \varrho^2\frac{\partial e_0}{\partial\varrho} \text{ and } p_c := \varrho^2\frac{\partial\hat{e}}{\partial\varrho}$$

where p_0 is the classical thermodynamic pressure and p_c can be interpreted as capillary pressure due to inhomogeneous density fields. The non-viscous stress turns to

$$\tilde{\mathbf{T}}^c = -\varrho\frac{\partial\hat{e}}{\partial\boldsymbol{z}} \otimes \nabla\varrho + \varrho\operatorname{div}(\varrho\frac{\partial\hat{e}}{\partial\boldsymbol{z}})\mathbf{I} - p_0\mathbf{I} - \varrho^2\frac{\partial\hat{e}}{\partial\varrho}\mathbf{I} = \mathbf{T}^c - p_0\mathbf{I}$$

where we call $\mathbf{T}^c := \tilde{\mathbf{T}}^c + p_0\mathbf{I}$ the capillary stress.

We will now turn our attention to a slightly more specific class of internal energies than (4.1) to obtain a hierarchy of Korteweg models. We will additionally find for each model a non-classical but simplified representation of $\operatorname{div}\mathbf{T}^c$. In the considerations below, we consider the capillary energy to be given by

$$\hat{e} = \frac{1}{2+\alpha}A(\varrho)\,|\nabla\Psi(\varrho)|^{2+\alpha}\,,$$

which leads to the final general form of the capillary stress written as

$$(4.2) \quad \mathbf{T}^c = -\varrho A(\varrho) \left|\nabla\Psi(\varrho)\right|^\alpha \nabla\Psi(\varrho) \otimes \nabla\Psi(\varrho) + \varrho \operatorname{div}\left(\varrho A(\varrho)\Psi'(\varrho) \left|\nabla\Psi(\varrho)\right|^\alpha \nabla\Psi(\varrho)\right) \mathbf{I}$$

$$- \frac{1}{2+\alpha} \varrho^2 \frac{\partial}{\partial\varrho}\left(A(\varrho) \left|\Psi'(\varrho)\right|^{2+\alpha}\right) \left|\nabla\varrho\right|^{2+\alpha} \mathbf{I}.$$

Example 4.1. *Specialization for $\alpha = 0$, $\Psi(\varrho) = \varrho$ and $A(\varrho) = \sigma\varrho^{-1}$*
  We quickly infer from (4.2) the relation

$$\mathbf{T}^c = -\sigma\nabla\varrho \otimes \nabla\varrho + \sigma\varrho\Delta\varrho\mathbf{I} + \frac{\sigma}{2} \left|\nabla\varrho\right|^2 \mathbf{I}.$$

The first term on the right hand side is the classical capillary tensor, which is often called Korteweg tensor. We emphasize that this model is almost the same as the one derived by Korteweg himself. With the help of the general equality

$$(4.3) \qquad \operatorname{div}\left(\nabla\psi \otimes \nabla\psi\right) = \Delta\psi\nabla\psi + \frac{1}{2}\nabla\left|\nabla\psi\right|^2 \quad \textit{for } \psi \textit{ smooth enough}$$

the divergence of this tensor is

$$(4.4) \qquad\qquad\qquad \operatorname{div}\mathbf{T}^c = \varrho\nabla\Delta\varrho.$$

From the mathematical point of view, it is easier to study (4.4) than the the pure Korteweg tensor $-\sigma\nabla\varrho \otimes \nabla\varrho$. In especially (4.4) leads to improved estimates on the solutions that cannot be obtained for the simple model. To emphasize this point, note that in the mathematical theory of weak solutions, the momentum equation is multiplied by $\boldsymbol{v}$ and integrated over space to obtain some estimates on the solutions. In particular, on may calculate [4]

$$\int_{\mathbb{R}^3} -\boldsymbol{v} \operatorname{div}\mathbf{T}^c = \int_{\mathbb{R}^3} -\boldsymbol{v}\varrho\nabla\Delta\varrho = \int_{\mathbb{R}^3} -\partial_t\varrho\Delta\varrho = \frac{d}{dt}\int_{\mathbb{R}^3} \frac{1}{2}\left|\nabla\varrho\right|^2.$$

This may lead to an estimate of the form $\|\nabla\varrho\|_{L^\infty(0,T;L^2(\mathbb{R}^n))} \leq C < \infty$. Due to the last observation, for each of the following examples we aim to find a formulation similar to (4.4). Bresch and Desjardins later on in [2] generalized (4.4) to a model which will be obtained in the next step.

Example 4.2. *Specialization for $\alpha = 0$ and $A(\varrho) = \sigma\varrho^{-1}$*
  Like in the first example, we quickly calculate

$$\mathbf{T}^c = -\sigma\nabla\Psi(\varrho) \otimes \nabla\Psi(\varrho) + \sigma\varrho \operatorname{div}(\Psi'(\varrho)\nabla\Psi(\varrho))\mathbf{I}$$

$$- \frac{1}{2}\sigma\varrho^2 \frac{\partial}{\partial\varrho}(\varrho^{-1}\left|\Psi'(\varrho)\right|^2) \left|\nabla\varrho\right|^2 \mathbf{I}$$

$$(4.5) \qquad = -\sigma\nabla\Psi(\varrho) \otimes \nabla\Psi(\varrho) + \sigma\varrho\Psi'(\varrho)\Delta\Psi(\varrho))\mathbf{I} + \frac{1}{2}\sigma\left|\nabla\Psi(\varrho)\right|^2 \mathbf{I}$$

This is the stress tensor considered in [2]. As in Example 4.1 it can be easily calculated that

$$(4.6) \qquad\qquad\qquad \operatorname{div}\mathbf{T}^c = \varrho\nabla\left(\Psi'(\varrho)\Delta\Psi(\varrho)\right)$$

Like (4.4), equation (4.6) leads to good additional estimates on ϱ. We highlight that [2] were motivated by mathematical properties of the arising system, while in our approach the model drops out from physical calculations. It may therefore reflect our intuition that "correct physics should end up in beautiful mathematics". (K.R. Rajagopal)

Example 4.3. *Specialization for $\alpha = 0$ and $A(\varrho) = \sigma\varrho^{-1}$ and $\Psi(\varrho) = \ln\varrho$*
   We infer from (4.5)

$$
\begin{aligned}
\mathbf{T}^c &= -\sigma\nabla\ln\varrho \otimes \nabla\ln\varrho + \sigma\Delta\ln\varrho + \mathbf{I} + \frac{1}{2}\sigma\left|\nabla\ln(\varrho)\right|^2\mathbf{I} \\
&= -\sigma\nabla\ln\varrho \otimes \nabla\ln\varrho + \frac{\sigma}{\varrho}\Delta\varrho + \mathbf{I} - \frac{1}{2}\sigma\left|\nabla\ln(\varrho)\right|^2\mathbf{I}.
\end{aligned}
$$

This model was studied in [6] where it was derived from the classical formula 4.9. It may be considered as a model in which the system tries to minimize relative gradients $\frac{\nabla\varrho}{\varrho}$ instead of absolute gradients $\nabla\varrho$.

   Of course, the latter model can also be obtained by the choice $A(\varrho) = \sigma\varrho^{-3}$ and $\Psi(\varrho) = \varrho$ or by putting $\kappa(\varrho) = \sigma\varrho^{-2}$ in (4.9) below, like it was obtained in [6]. However, the explanation in our setting gives more insight into the physical assumptions which are implied in this model.

Example 4.4. *Specialization for $\alpha = 0$*
   We now want to generalize (4.6) *even more. In the case under consideration, the capillary stress simplifies to*

$$
\begin{aligned}
\mathbf{T}^c &= -\frac{1}{2}\varrho^2\frac{\partial}{\partial\varrho}\left(A(\varrho)\left|\Psi'(\varrho)\right|^2\right)\left|\nabla\varrho\right|^2\mathbf{I} + \varrho\operatorname{div}(\varrho A(\varrho)\Psi'(\varrho)\nabla\Psi(\varrho))\mathbf{I} \\
&\quad -\varrho A(\varrho)\nabla\Psi(\varrho) \otimes \nabla\Psi(\varrho) \\
&= \frac{1}{2}\varrho^2 A'(\varrho)\left|\nabla\Psi(\varrho)\right|^2\mathbf{I} + \varrho A(\varrho)\left|\nabla\Psi(\varrho)\right|^2\mathbf{I} + \varrho^2 A(\varrho)\Psi'(\varrho)\Delta\Psi(\varrho)\mathbf{I} \\
&\quad -\varrho A(\varrho)\nabla\Psi(\varrho) \otimes \nabla\Psi(\varrho).
\end{aligned}
$$

With the help of (4.3) *and*

$$
(4.7) \qquad (\nabla\psi(\varrho) \otimes \nabla\psi(\varrho))\nabla\phi(\varrho) = (\phi'\psi'\psi')(\varrho)\left|\nabla\varrho\right|^2\nabla\varrho = \left|\nabla\psi(\varrho)\right|^2\nabla\phi(\varrho)
$$

the divergence of the capillary stress can be calculated as

$$
\begin{aligned}
\operatorname{div}\mathbf{T}^c &= \nabla\left(\frac{1}{2}\varrho^2 A'(\varrho)\left|\nabla\Psi(\varrho)\right|^2\right) + \frac{1}{2}\varrho A(\varrho)\nabla\left|\nabla\Psi(\varrho)\right|^2 \\
&\quad -\varrho A(\varrho)\nabla\Psi(\varrho)\Delta\Psi(\varrho) + \nabla\left(\varrho^2 A(\varrho)\Psi'(\varrho)\Delta\Psi(\varrho)\right) \\
(4.8) \qquad &= \nabla\left(\frac{1}{2}\varrho^2 A'(\varrho)\left|\nabla\Psi(\varrho)\right|^2\right) + \frac{1}{2}\varrho A(\varrho)\nabla\left|\nabla\Psi(\varrho)\right|^2 + \varrho\nabla\left(\varrho A(\varrho)\Psi'(\varrho)\Delta\Psi(\varrho)\right).
\end{aligned}
$$

Of course, inserting $A(\varrho) = \sigma\varrho^{-1}$ evidently yields (4.6) *again. An other interesting specialization of this model is the case $\Psi(\varrho) = \varrho$ resulting in*

$$
\mathbf{T}^c = \frac{1}{2}\varrho^2 A'(\varrho)\left|\nabla\varrho\right|^2\mathbf{I} + \varrho A(\varrho)\left|\nabla\varrho\right|^2\mathbf{I} + \varrho^2 A(\varrho)\Delta\varrho\mathbf{I} - \varrho A(\varrho)\nabla\varrho \otimes \nabla\varrho.
$$

For the special choice $A(\varrho) = \frac{\kappa(\varrho)}{\varrho}$ the latter expression for $\mathbf{T}^c$ becomes

$$
(4.9) \qquad \mathbf{T}^c = \frac{1}{2}\left(\kappa(\varrho) + \varrho\kappa'(\varrho)\right)\left|\nabla\varrho\right|^2\mathbf{I} + \varrho\kappa(\varrho)\Delta\varrho\mathbf{I} - \kappa(\varrho)\nabla\varrho \otimes \nabla\varrho
$$

which is also used in literature (we refer to [6] and the references therein).

We see, that the first two terms in (4.8) in general do not cancel out and the analysis as well as the numerical simulations of such a system will be more complicated than in the traditional model of example 4.1. To our knowledge, such systems have not been studied in literature before.

Example 4.5. *Specialization for* $\Psi(\varrho) = \varrho$ *and* $\alpha \neq 0$
For the specified specialization, (4.2) turns into

$$
\begin{aligned}
\mathbf{T}^c &= -\varrho A(\varrho) |\nabla \varrho|^\alpha \nabla \varrho \otimes \nabla \varrho + \varrho \operatorname{div}(\varrho A(\varrho) |\nabla \varrho|^\alpha \nabla \varrho)\mathbf{I} \\
&\quad -p_0 \mathbf{I} - \frac{1}{2+\alpha} \varrho^2 A'(\varrho) |\nabla \varrho|^{2+\alpha} \mathbf{I} \\
&= -\varrho A(\varrho) |\nabla \varrho|^\alpha \nabla \varrho \otimes \nabla \varrho + \varrho A(\varrho) |\nabla \varrho|^{2+\alpha} \mathbf{I} \\
&\quad + \frac{1+\alpha}{2+\alpha} \varrho^2 A'(\varrho) |\nabla \varrho|^{2+\alpha} \mathbf{I} + \varrho^2 A \operatorname{div}\left(|\nabla \varrho|^\alpha \nabla \varrho\right).
\end{aligned}
$$

We make use of (4.7) and replace (4.3) by

$$
\operatorname{div}\left(|\nabla \psi|^\alpha \nabla \psi \otimes \nabla \psi\right) = \operatorname{div}\left(|\nabla \psi|^\alpha \nabla \psi\right) \nabla \psi + \frac{1}{2+\alpha} \nabla |\nabla \psi|^{2+\alpha}
$$

to obtain

$$
\operatorname{div} \mathbf{T}^c = \frac{1+\alpha}{2+\alpha} \nabla\left(\varrho^2 A'(\varrho) |\nabla \varrho|^{2+\alpha}\right) + \frac{1+\alpha}{2+\alpha} \varrho A(\varrho) \nabla |\nabla \varrho|^{2+\alpha} + \varrho \nabla\left(\varrho A(\varrho) \operatorname{div}\left(|\nabla \varrho|^\alpha \nabla \varrho\right)\right)
$$

To our knowledge, the latter example is not studied in literature, although it seems to be very interesting from the modeling as well as from the mathematical point of view. For the specific choice $A(\varrho) = \sigma \varrho^{-1}$, it turns to

$$
\operatorname{div} \mathbf{T}^c = \sigma \varrho \nabla\left(\operatorname{div}\left(|\nabla \varrho|^\alpha \nabla \varrho\right)\right)
$$

which, according to the calculations in the first example, leads to

$$
\int_{\mathbb{R}^3} -\boldsymbol{v} \operatorname{div} \mathbf{T}^c = \frac{d}{dt} \int_{\mathbb{R}^3} \frac{1}{2+\alpha} |\nabla \varrho|^{2+\alpha}
$$

4.1. Granular materials steady flow. We will now consider a granular material steady flow due to a constant force $f = f(x)$ between two infinite parallel plates oriented parallel to the (x, z)-plane with a distance y_0. The force is assumed to take the form $f = (C_0 x, 0, 0)$ and the velocity is assumed to take the form $\boldsymbol{v} = (\boldsymbol{v}_1(y), 0, 0)$. Since in the steady case $\partial_t \varrho = 0$ and $\partial_t \boldsymbol{v} = 0$, the mass balance equation leads $\boldsymbol{v}_1(y)\partial_x \varrho = 0$ which is $\partial_x \varrho = 0$. We therefore obtain for the total stress in the most simple case

$$
\mathbf{T} = \begin{bmatrix} P & \mu\, \boldsymbol{v}_1'(y) & \\ \mu\, \boldsymbol{v}_1'(y) & P - \sigma\left(\partial_y \varrho\right) & -\sigma \partial_y \varrho\, \partial_z \varrho \\ & -\sigma \partial_y \varrho\, \partial_z \varrho & P - \sigma\left(\partial_z \varrho\right)^2 \end{bmatrix}
$$

with $P := -p_0 + \sigma \varrho \Delta \varrho \mathbf{I} + \frac{1}{2}\sigma |\nabla \varrho|^2 \mathbf{I}$. Then, the material exhibits some normal stress differences which read

$$
\mathbf{T}_{11} - \mathbf{T}_{22} = \sigma\left(\partial_y \varrho\right)^2, \quad \mathbf{T}_{22} - \mathbf{T}_{33} = \sigma\left(\partial_z \varrho\right)^2, \quad \mathbf{T}_{33} - \mathbf{T}_{11} = -\sigma\left(\partial_z \varrho\right)^2.
$$

On the other hand, it is also clear that a dependence of μ on $\mathbf{D} \cdot \mathbf{D}$ would lead to shear thickening or shear thinning behavior.

For the sake of simplicity, we will now focus on a density field which is independent on z, i.e. $\varrho = \varrho(y)$. Our governing set of equations for the steady state is then div $\mathbf{T} + f = 0$ which splits up into the following three equations:

$$\partial_x p = \mu \, \mathbf{v}_1'' + C_0, \quad \partial_y p + \partial_y \left(\sigma \varrho \partial_y^2 \varrho + \frac{\sigma}{2} \left| \partial_y \varrho \right|^2 \right), \quad \partial_z p = 0.$$

The first equation shows, that $\partial_x(\partial_x p - f_1'(x)) = 0$ and all three equations together finally yield for the pressure

$$p(x, y) = (C_0^* + C_0) \, x + C_1 - \left(\sigma \varrho \partial_y^2 \varrho + \frac{\sigma}{2} \left| \partial_y \varrho \right|^2 \right).$$

The velocity profile $\mathbf{v}_1$ takes a parabolic shape, where we have to put in the velocity on the boundary, but the density distribution cannot be determined without knowledge on the pressure field and vice versa. From out physical ansatz it is reasonable to assume $p(x, y) = (C_0^* + C_0) \, x + p_0(\varrho(y))$ and to solve the second order ODE for ϱ. Remark that in the latter case, the two constants $C_0^* + C_0$ and C_1 have to be prescribed in order to get a unique solution. The shape of $\mathbf{v}_1(y)$ basically depends on the value of C_0, i.e. on the force which is applied to the material.

4.2. **Numerical simulations for the distribution of ϱ in equilibrium.** Maybe perform computations in Equilibrium, i.e. $\mathbf{v} = 0$, which leads to div $\mathbf{T}^c = 0$ and solve this on a square $[0, 1]^2$ with $\varrho(0, y) = 1$, $\varrho(1, y) = 0.01$ and appropriate (have to think over it) conditions on $[x, 0]$ and $[x, 1]$.

5. Concluding remarks

Summarize what has been done.

We use a very simple form for the rate of entropy production

We assume the constitutive equation for ξ so that in general ξ may depend on ϱ, θ and both thermodynamic fluxes and thermodynamic affinities. Requiring that the dependence on thermodynamic fluxes is convex, we obtain the constitutive equation involving the Cauchy stress by maximizing ξ w.r.t. the thermodynamic fluxes that cause the deformation and consider the other quantities as parameters. The maximization of ξ is complemented by the requirement that (3.7) holds.

References

[1] D. M. Anderson, G. B. McFadden, and A. A. Wheeler. Diffuse-interface methods in fluid mechanics. *Annual review of fluid mechanics*, 30:139–165, 1998.

[2] D. Bresch and B. Desjardins. Quelques modèles diffusifs capillaires de type Korteweg. *Comptes Rendus Mecanique*, 332(11):881–886, November 2004.

[3] H. Callen. *Thermodynamics and an introduction to thermostatics.* Wiley, London, 1985.

[4] R. Danchin and B. Desjardins. Existence of solutions for compressible fluid models of Korteweg type. *Annales de l'Institut Henri Poincare (C) Non Linear Analysis*, 18(1):97–133, 2001.

[5] J. E. Dunn and J. Serrin. On the thermomechanics of interstitial working. *Arch. Rational Mech. Anal.*, 88:95–133, 1985.

[6] B. Haspot. Existence of global weak solution for compressible fluid models of Korteweg type. to appear in Journal of Mathematical Fluid Mechanics, DOI:10.1007/s00021-009-0013-2, 2010.

[7] D. J. Korteweg. Sur la forme que prennent les équations du mouvement des fluides si l'on tient compte des forces capillaires causées par des variations de densité considérables mais continues et sur la théorie de la capillarité dans l'hypothèse d'une variation continue de la densité. *Archives Néerlandaises des sciences exactes et naturelles. Ser 2*, 6:1–24, 1901.

[8] J. Málek and K. R. Rajagopal. On the modeling of inhomogeneous incompressible fluid-like bodies. *Mechanics of Materials*, 38:233–242, 2006.

[9] J. Málek and K. R. Rajagopal. Compressible generalized Newtonian fluids. *Z. Angew. Math. Phys.*, 61:DOI 10.1007/s00033–010–0061–8, 2010.

[10] M. M. Mehrabadi, S. C. Cowin, and M. Massoudi. Conservation laws and constitutive relations for density-gradient-dependent viscous fluids. *Continuum Mechanics and Thermodynamics*, 17(2):183–200, May 2005.

[11] K. R. Rajagopal. The elasticity of elasticity. *Z. Angew. Math. Phys.*, 58(2):309–317, 2007.

[12] K. R. Rajagopal and A. R. Srinivasa. On thermomechanical restrictions of continua. *Proc. R. Soc. Lond. A*, 460:631–651, 2004.

[13] K. R. Rajagopal and A. R. Srinivasa. On the thermodynamics of fluids defined by implicit constitutive relations. *Z. Angew. Math. Phys.*, 59:715–729, 2008.

[14] C. Truesdell and W. Noll. *The non-linear field theories of mechanics*, volume 1. Springer, Berlin, Heidelberg, 1991. 3nd edition (edited by S. Antmann).

[15] J. D. Van der Waals. Théorie thermodynamique de la capillarité, dans l'hypothèse d'une variation continue de la densité. *Archives Néerlandaises des sciences exactes et naturelles.*, XXVIII:121–209, 1893.

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