Internal variables as a tool for extending Navier–Stokes equations

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Abstract

The formalism of the internal variables theory is applied to extend Navier–Stokes equations. The internal variables theory provides a thermodynamically consistent derivation of constitutive relations and equations of motion without *a priory* specification of the nature of the variables. Both single and dual internal variables cases are considered in detail. The similarity and differences of the approaches are clearly indicated. In the single internal variable framework, the elimination of the internal variable provides Maxwell-type constitutive relations and hyperbolic equations of motion. The dual internal variable approach allows us to obtain even more complicated models of fluid flow, which contain coupled equations for fluid motion and internal variable evolution.

1 Introduction

The Navier–Stokes equations constitute the cornerstone of computational fluid dynamics [1-3]. As for every good mathematical model, these equations are valid for idealized processes. For more complex situations the Navier–Stokes equations need to be extended. Various methods have been used for such an extension, as it is reviewed in books by Joseph [4], Beris and Edwards [5], and Deville and Gatski [6]. It should be noted that any extension of the Navier-Stokes equations is associated with the introduction of additional variables. For instance, Brenner [7, 8] taken mass diffusion into account, Peshkov and Romenski [9] introduced elastic distortion, Hu and Racke [10] applied Maxwell's relaxation, fluxes are used as additional independent state variables in extended irreversible thermodynamics [11] and in rational extended thermodynamics [12]. Application of internal variables is natural in this context. The use of internal variables for the extension of Navier–Stokes equations has a long history. Kluitenberg [13, 14] called the corresponding variables as "internal degrees of freedom". Lebon [15] allowed the dependence of the Gibbs equation on "extra variables" though the notion of internal variables was already well known [16]. "Hidden variables" in a viscous fluid model appeared in papers by Morro [17] and Bampi and Morro [18]. Dashner and VanArsdale [19] used an "internal deformation tensor", and additional state variables were introduced by Grmela [20, 21] for the generalization of hydrodynamic equations. Internal variables per se were

used by Maugin and Drouot [22–24] for the modelling of complex fluids flow. Fluids with internal degrees of freedom were considered in [25, 26] from the point of view of the extended irreversible thermodynamics. A comprehensive review of the application of internal variables to fluid flows was given in the paper by Maugin and Muschik [27] and in the book by Beris and Edwards [5]. An auxiliary variable related to irreversible changes on the microstructure was introduced in [28, 29] to formulate constitutive models for fluids.

It should be noted that the standard internal variable theory [30–32] provides a thermodynamically consistent description of the influence of a possible material microstructure. Recently, the internal variables approach was generalized exploiting the further enlargement of the thermodynamic state space [33–35]. The dual internal variable concept was successfully applied for generalized elasticity and heat conduction description [34, 36, 37]. It is worth, therefore, to employ the full internal variables framework for the extension of classical equations of fluid motion. This framework is based on the exploitation of the dissipation inequality. Though only linear solution of the dissipation inequality is considered in the paper, it is demonstrated that the elimination of internal variable in the single internal variable theory recovers existing Maxwell-type constitutive models which are commonly postulated in advance. The main result of the paper follows from the application of the dual internal variable concept resulting in the derivation of coupled equations for fluid motion and internal variable evolution.

The paper starts with the reminder of basic balance laws and constitutive relations for classical hydrodynamics (Sect. 2). The single internal variable theory is applied to the hydrodynamic description in Sect. 3. The specific case of the independence of the free energy density of the gradient of the internal variable is considered in Sect.4. It is shown that the elimination of the internal variable provides Maxwell-type constitutive relations and hyperbolic equations of motion. The dual internal variable approach presented in Sect. 5 allows to obtain even more complicated models of fluid flow, which contain coupled equations for fluid motion and internal variable evolution. Conclusions are formulated in Sect.6.

2 Background: balance laws and constitutive relations

The motion of a continuous medium is characterized by balance laws. In the Eulerian (spatial) representation, the local balance laws can be represented as follows (cf. [38]):

• conservation of mass

$$\rho_t + \rho \operatorname{div} \mathbf{v} = 0, \tag{1}$$

where ρ is the density field, **v** is the velocity field, subscript t denotes the material time derivative.

• balance of linear momentum

$$\rho \mathbf{v}_t - \operatorname{div} \boldsymbol{\sigma} = \rho \mathbf{f},\tag{2}$$

where σ is the Cauchy stress tensor, **f** is a body force.

• balance of angular momentum

$$\boldsymbol{\sigma}^T = \boldsymbol{\sigma},\tag{3}$$

where upper index T denotes transposition.

• balance of energy

$$\rho e_t - \boldsymbol{\sigma} : \mathbf{D} - \operatorname{div} \mathbf{q} = \rho h, \tag{4}$$

where e is the internal energy density, θ is temperature field, **D** is the strain rate tensor, **q** is heat flux, and h is a heat body source.

The balance laws are complemented by the entropy inequality

$$\rho\eta_t + \operatorname{div}\left(\frac{\mathbf{q}}{\theta}\right) - \rho\frac{h}{\theta} \ge 0,\tag{5}$$

where η is the entropy density field.

For fluids, the free energy density $\psi = e - \eta \theta$ depends on matter density ρ , the strain rate tensor **D**, temperature θ , and its gradient $\nabla \theta$

$$\psi = \psi(\rho, \mathbf{D}, \theta, \nabla\theta). \tag{6}$$

Constitutive relations should satisfy the Clausius–Duhem inequality (no body sources) [39]

$$-\rho\psi_t - \rho\eta\theta_t - \frac{\mathbf{q}}{\theta} \cdot \nabla\theta + \boldsymbol{\sigma} : \mathbf{D} \ge 0.$$
(7)

The standard consideration leads to the definition of entropy

$$\eta = -\frac{\partial\psi}{\partial\theta},\tag{8}$$

and to the independence of the free energy density of the strain rate tensor and the temperature gradient

$$\frac{\partial \psi}{\partial \mathbf{D}} = \mathbf{0}, \quad \frac{\partial \psi}{\partial \nabla \theta} = \mathbf{0}.$$
 (9)

The thermodynamic pressure p is defined by [39]

$$p = \rho^2 \frac{\partial \psi}{\partial \rho}.\tag{10}$$

The constitutive relation for the stress in a compressible, linearly viscous (Newtonian) fluid has the form

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\mu\mathbf{D} + \lambda(\mathrm{tr}\mathbf{D})\mathbf{I},\tag{11}$$

with the dilatational viscosity, λ and the shear viscosity, μ . In general, the viscosity coefficients may depend on the density and temperature. In this paper, these coefficients are considered as constants.

Equations of motion follow from balances of mass and momentum (in the absence of body sources) [2]

$$\rho_t = \rho \operatorname{div} \mathbf{v}, \tag{12}$$

$$\rho \mathbf{v}_t = -\nabla p + \mu \Delta \mathbf{v} + (\lambda + \mu) \nabla (\operatorname{div} \mathbf{v}).$$
(13)

These equations are generally referred to as the compressible Navier–Stokes equations. Thermal contribution is governed by the Fourier law

$$\mathbf{q} = -k\nabla\theta, \quad k \ge 0,\tag{14}$$

where k is the thermal conductivity.

3 Single internal variable framework

The Navier–Stokes equations are valid for homogeneous isotropic fluids. To include into consideration more complicated cases, we apply the internal variable formalism. In the single internal variable theory, the state space is expanded by means of an internal variable α and its gradient $\nabla \alpha$ [40, cf.]. This means that the free energy density depends on the density ρ , temperature θ , the internal variable α and its gradient $\nabla \alpha$

$$\psi = \psi(\rho, \theta, \alpha, \nabla \alpha). \tag{15}$$

The nature of the internal variable is not prescribed in advance. Nevertheless, it is possible to derive an evolution equation of the internal variable in a general form using the dissipation inequality (7). In fact, the material time derivative of the free energy density is calculated using the chain rule

$$\psi_t = \frac{\partial \psi}{\partial \rho} \rho_t + \frac{\partial \psi}{\partial \theta} \theta_t + \frac{\partial \psi}{\partial \alpha} \alpha_t + \frac{\partial \psi}{\partial \nabla \alpha} (\nabla \alpha)_t.$$
(16)

Introducing the definitions

$$\mathbf{A} := -\frac{\partial \psi}{\partial \boldsymbol{\alpha}}, \quad \mathcal{A} := -\frac{\partial \psi}{\partial \nabla \boldsymbol{\alpha}}, \tag{17}$$

we can rewrite Clausius–Duhem inequality (7) as follows:

$$-\rho \frac{\partial \psi}{\partial \rho} \rho_t + \mathbf{A} : (\nabla \boldsymbol{\alpha})_t - \frac{\mathbf{q}}{\theta} \cdot \nabla \theta + \boldsymbol{\sigma} : \mathbf{D} \ge 0.$$
(18)

Taking into account the material time derivative of the density

$$\rho_t = -\rho \mathbf{I} : \mathbf{D},\tag{19}$$

and using pressure relation (10), we represent dissipation inequality (7) in the form of a linear combination of products of thermodynamic fluxes and forces

$$(p\mathbf{I} + \boldsymbol{\sigma}) : \mathbf{D} + \mathbf{A} : \boldsymbol{\alpha}_t + \boldsymbol{\mathcal{A}} : (\nabla \boldsymbol{\alpha})_t - \frac{\mathbf{q}}{\theta} \cdot \nabla \theta \ge 0.$$
(20)

The obtained dissipation inequality is the basis for the derivation of the evolution equation for the internal variable. Different approaches are used to exploit the dissipation inequality [41]. The most known is the Coleman-Noll procedure [42]. In this procedure, the Clausius-Duhem inequality is presumed to hold for any choice of the time rate of the state variables. For any fixed state, it is supposed that the time rates are chosen arbitrarily. Due to the arbitrariness and independency of \mathbf{D} , $\boldsymbol{\alpha}_t$, and $(\nabla \boldsymbol{\alpha})_t$,

$$\boldsymbol{\sigma} = p\mathbf{I}, \quad \mathbf{A} = \mathcal{A} = \mathbf{0}, \tag{21}$$

i.e., the free energy density must be independent of α .

It should be noted that the assumption of arbitrariness and independency between **D** and α_t is not applicable in the case of internal variables of state because they are "observable but not controllable" according to the Bridgman– Kestin insight [32, 43, 44]. The arbitrariness and independence is true for internal degrees of freedom which, in contrast to internal variables of state, are measurable and controllable by means of corresponding applied forces in volume and at surfaces [32, 44].

Another method of the exploitation of the dissipation inequality was proposed by Liu [45]. The difference between Coleman–Noll and Liu procedures is based on the definition of the entropy flux [46]. The Coleman–Noll and Liu procedures are equivalent in simple systems [47], but not equivalent if the material is not simple [41, 48]. The Liu procedure has been applied successfully to weakly non-local thermomechanical theory [49–53]. However, the Liu procedure is also based on the arbitrariness and independence of state variables [45].

Fortunately, in case of internal variables it is possible to derive the complete evolution equations using thermodynamic forces and fluxes relationships [41, 54]. Keeping in mind the extension of the internal variables theory [33], we apply the Onsager procedure for the solution of the Clausius-Duhem inequality.

3.1 Isothermal case

To be as simple as possible we consider the isothermal case. In this case, dissipation inequality (20) is reduced to

$$(p\mathbf{I} + \boldsymbol{\sigma}) : \mathbf{D} + \mathbf{A} : \boldsymbol{\alpha}_t + \boldsymbol{\mathcal{A}} : (\nabla \boldsymbol{\alpha})_t \ge 0,$$
(22)

and the thermodynamic fluxes and forces are identified as presented in Table 1.

The linear solution of dissipation inequality (22) is given by

$$\begin{pmatrix} p\mathbf{I} + \boldsymbol{\sigma} \\ \boldsymbol{\alpha}_t \\ (\nabla \boldsymbol{\alpha})_t \end{pmatrix}$$
(23)

	Flux	Force
Mechanical	$p\mathbf{I} + \boldsymbol{\sigma}$	D
Internal	$oldsymbol{lpha}_t$	A
Internal	$(\nabla \boldsymbol{lpha})_t$	\mathcal{A}

Table 1: Thermodynamic fluxes and forces in the isothermal case.

i.e.,

$$p\mathbf{I} + \boldsymbol{\sigma} = M_{11}\mathbf{D} + M_{12}\mathbf{A} + M_{13}\mathcal{A}, \qquad (24)$$

$$\boldsymbol{\alpha}_t = M_{21}\mathbf{D} + M_{22}\mathbf{A} + M_{23}\mathcal{A} \tag{25}$$

$$(\nabla \boldsymbol{\alpha})_t = M_{31}\mathbf{D} + M_{32}\mathbf{A} + M_{33}\mathcal{A}$$
(26)

where components M_{ij} of the matrix **M** are considered as constants for simplicity. The nonnegativity of the entropy production results in the positive semidefiniteness of the symmetric part of the matrix **M**, which requires [55, 56]

$$M_{11} \ge 0, \quad M_{22} \ge 0, \quad M_{11}M_{22} - \frac{(M_{12} + M_{21})^2}{2} \ge 0.$$
 (27)

The symmetry of coefficients in the Onsagerian matrix \mathbf{M} is not necessary [53]. Relationships (24) and (25) determine thermodynamically consistent constitutive relation and the evolution equation for the internal variable, respectively. These relationships are not prescribed *a priory* or phenomenologically, but they are consequences of the dissipation inequality in the framework of the single internal variable theory.

The next step is the specification of the dependence of the free energy density on the internal variable and its gradient. In the case of a quadratic dependence

$$\psi(\dots, \alpha, \nabla \alpha) = \dots + \frac{B}{2}\alpha^2 + \frac{C}{2}(\nabla \alpha)^2, \qquad (28)$$

the contribution of the internal variable in the right-hand side of Eqs. (24)–(25) is

$$\mathbf{A} - \operatorname{div} \mathcal{A} = -B\boldsymbol{\alpha} + C\Delta\boldsymbol{\alpha}.$$
 (29)

This leads to the Ginzburg–Landau-type equation for the evolution of the internal variable

$$\boldsymbol{\alpha}_{t} = M_{21}\mathbf{D} + M_{22}\left(-B\boldsymbol{\alpha} + C\Delta\boldsymbol{\alpha}\right).$$
(30)

The internal variable α still remains unspecified.

3.2 Elimination of internal variable

Remarkably, there is no need to set the internal variable explicitly, because it can be eliminated from the solution of the dissipation inequality. In fact, after the rearrangement of Eq. (25) using (24), we have

$$\boldsymbol{\alpha}_{t} = M_{21}\mathbf{D} + \frac{M_{22}}{M_{12}}\left(p\mathbf{I} + \boldsymbol{\sigma} - M_{11}\mathbf{D}\right).$$
(31)

The material time derivative of relation (24) results in

$$p_t \mathbf{I} + \boldsymbol{\sigma}_t = M_{11} \mathbf{D}_t + M_{12} \left(-B\boldsymbol{\alpha}_t + C\Delta\boldsymbol{\alpha}_t \right).$$
(32)

Substituting the time derivative of internal variable (31) into relationship (32), we obtain after some algebra

$$\left(p\mathbf{I} + \boldsymbol{\sigma} - \frac{\det M}{M_{22}}\mathbf{D}\right) + \frac{1}{M_{22}B}\left(p_t\mathbf{I} + \boldsymbol{\sigma}_t - M_{11}\mathbf{D}_t\right) = \frac{C}{B}\Delta\left(p\mathbf{I} + \boldsymbol{\sigma} - \frac{\det M}{M_{22}}\mathbf{D}\right)$$
(33)

The elimination of the internal variable represents the solution of the dissipation inequality as the combination of three clearly distinctive parts. The influence of the internal variable manifests itself in the structure of the relationship (33) and in the values of coefficients B and C in the quadratic dependence of the free energy density (28). It is instructive to consider limit cases of values of the coefficients.

3.3 Limit cases

3.3.1 Case 1: B = 0.

In this case, the free energy density is independent of the internal variable α . This independence results in the constitutive relation for the stress tensor in the form

$$p_t \mathbf{I} + \boldsymbol{\sigma}_t - M_{11} \mathbf{D}_t = C M_{22} \Delta \left(p \mathbf{I} + \boldsymbol{\sigma} - \frac{\det M}{M_{22}} \mathbf{D} \right).$$
(34)

The obtained relationship corresponds to the parabolic evolution of the constitutive relation.

3.3.2 Case 2: $B \rightarrow \infty$.

High values of B lead to the simple constitutive relation

$$p\mathbf{I} + \boldsymbol{\sigma} - \frac{\det M}{M_{22}}\mathbf{D} = 0, \qquad (35)$$

which match with that for the classical Newtonian fluid.

3.3.3 Case 3: $C \to \infty$.

In this case, the Laplacian of the previous relationship is zero, which does not give an essential generalization

$$\Delta \left(p\mathbf{I} + \boldsymbol{\sigma} - \frac{\det M}{M_{22}} \mathbf{D} \right) = 0.$$
(36)

3.3.4 Case 4: C = 0.

The free energy density is independent of the gradient of the internal variable in this case that leads to the extension of the classical constitutive relation for Newtonian fluids

$$\left(p\mathbf{I} + \boldsymbol{\sigma} - \frac{\det M}{M_{22}}\mathbf{D}\right) + \frac{1}{M_{22}B}\left(p_t\mathbf{I} + \boldsymbol{\sigma}_t - M_{11}\mathbf{D}_t\right) = 0.$$
 (37)

This case deserves a more detailed consideration.

4 Independence from the gradient of the internal variable

If the free energy is independent of the gradient of the internal variable, then

$$\mathbf{A} = -B\boldsymbol{\alpha}.\tag{38}$$

Representing each tensor in the sum of hydrostatic and deviatoric components, we note that their contributions into the dissipation inequality are orthogonal since $\mathbf{A}^h : \mathbf{B}^d = 0$ for arbitrary symmetric tensors. It follows that the solution of dissipation inequality (22) should be taken separately for the hydrostatic part (with the upper index h)

$$p\mathbf{I} + \boldsymbol{\sigma}^{h} = M_{11}^{h} \mathbf{D}^{s} + M_{12}^{h} \mathbf{A}^{h}, \qquad (39)$$

$$\boldsymbol{\alpha}^{h}{}_{t} = M^{h}_{21}\mathbf{D}^{h} + M^{h}_{22}\mathbf{A}^{h}, \qquad (40)$$

and for the deviatoric part (marked by the upper index d)

$$\boldsymbol{\sigma}^{d} = M_{11}^{d} \mathbf{D}^{d} + M_{12}^{d} \mathbf{A}^{d}, \qquad (41)$$

$$\boldsymbol{\alpha}^{d}{}_{t} = M_{21}^{d} \mathbf{D}^{d} + M_{22}^{d} \mathbf{A}^{d}.$$

$$\tag{42}$$

The elimination of the internal variable from the solution of the dissipation inequality in the hydrostatic case results in

$$p\mathbf{I} + \boldsymbol{\sigma}^{h} + \frac{1}{BM_{22}^{h}} \left(p_{t}\mathbf{I} + \boldsymbol{\sigma}_{t}^{h} \right) = \frac{M_{11}^{h}}{BM_{22}^{h}} \mathbf{D}_{t}^{h} + \frac{\det M^{h}}{M_{22}^{h}} \mathbf{D}^{h}.$$
 (43)

Similarly, for the deviatoric case the elimination of the internal variable gives

$$\boldsymbol{\sigma}^{d} + \frac{1}{BM_{22}^{d}}\boldsymbol{\sigma}_{t}^{d} = \frac{M_{11}^{d}}{BM_{22}^{d}}\mathbf{D}_{t}^{d} + \frac{\det M^{d}}{M_{22}^{d}}\mathbf{D}^{d}.$$
(44)

4.1 Limit case $B \to \infty$.

It is easy to see that in the limit case $B \to \infty$ relationships (43) and (44) are reduced to

$$p\mathbf{I} + \boldsymbol{\sigma}^{h} = \frac{\det M^{h}}{M_{22}^{h}} \mathbf{D}^{h}, \qquad (45)$$

and

$$\boldsymbol{\sigma}^{d} = \frac{\det M^{d}}{M_{22}^{d}} \mathbf{D}^{d}.$$
(46)

The sum of the last two equations

$$p\mathbf{I} + \boldsymbol{\sigma} = \left(\frac{\det M^h}{M_{22}^h} - \frac{\det M^d}{M_{22}^d}\right)\mathbf{D}^h + \frac{\det M^d}{M_{22}^d}\mathbf{D},\tag{47}$$

can be represented in the form of constitutive equation (11) for the Cauchy stress

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\mu\mathbf{D} + \lambda(\mathrm{tr}\mathbf{D})\mathbf{I},\tag{48}$$

after the identification of the values of coefficients as

$$\frac{\det M^d}{M_{22}^d} = 2\mu, \quad \left(\frac{\det M^h}{M_{22}^h} - \frac{\det M^d}{M_{22}^d}\right) = 3\lambda,$$

since $3\mathbf{D}^{h} = (\mathrm{tr}\mathbf{D})\mathbf{I}$ by definition. It is clear that the Navier–Stokes equations correspond to the considered limiting case.

4.2 Maxwell fluids

Now it is possible to see how the Navier–Stokes equations can be extended due to the presence of the internal variable. To simplify the matter, we set

$$M_{22}^d = M_{22}^h = M_{22}, \quad \tau = \frac{1}{BM_{22}}.$$

Combining Eqs. (43) and (44) we have

$$p\mathbf{I} + \boldsymbol{\sigma} - \frac{\det M^h}{M_{22}}\mathbf{D}^h - \frac{\det M^d}{M_{22}}\mathbf{D}^d - \tau \left(p_t\mathbf{I} + \boldsymbol{\sigma}_t - M_{11}^h\mathbf{D}_t^h - M_{11}^d\mathbf{D}_t^d\right).$$
(49)

This relationship can be represented as

$$p\mathbf{I} + \boldsymbol{\sigma} - 2\mu\mathbf{D} - \lambda \mathrm{tr}(\mathbf{D})\mathbf{I} = -\tau \left(p_t\mathbf{I} + \boldsymbol{\sigma}_t - 2\mu_1\mathbf{D}_t - \lambda_1 \mathrm{tr}(\mathbf{D})_t\mathbf{I}\right), \quad (50)$$

with the evident notation $M_{11}^d = 2\mu_1$, $M_{11}^h - M_{11}^d = \lambda_1$. Resolving Eq. (50) for the stress

$$\boldsymbol{\sigma} + \tau \boldsymbol{\sigma}_t = -p\mathbf{I} + 2\mu\mathbf{D} + \lambda \mathrm{tr}(\mathbf{D})\mathbf{I} - \tau \left(p_t\mathbf{I} - 2\mu_1\mathbf{D}_t - \lambda_1 \mathrm{tr}(\mathbf{D})_t\mathbf{I}\right), \quad (51)$$

we arrive at a generalization of the constitutive equation for Maxwell fluids which has a more complex structure in the comparison with early models [57, 58] as well as with recent research [10, 59–62]. Any invariant material time derivative can be used in Eq. (51) [4].

4.3 Equations of motion

The balance of linear momentum

$$\rho \mathbf{v}_t = \operatorname{div} \boldsymbol{\sigma},\tag{52}$$

requires the calculation of the divergence of the stress tensor. Applying divergence operator to Eq. (51)

$$\operatorname{div} \boldsymbol{\sigma} + \tau \operatorname{div} \boldsymbol{\sigma}_t = -\nabla p + 2\mu \Delta \mathbf{v} + (\lambda + \mu) \nabla (\operatorname{div} \mathbf{v}) - \tau \left(\nabla p_t - 2\mu_1 \Delta \mathbf{v}_t - (\lambda_1 + \mu_1) \nabla (\operatorname{div} \mathbf{v})_t \right),$$
(53)

we obtain a hyperbolic version of the Navier–Stokes equation (c.f. [63, 64])

$$\rho \mathbf{v}_t + \tau \rho \mathbf{v}_{tt} = -\nabla p + 2\mu \Delta \mathbf{v} + (\lambda + \mu) \nabla (\operatorname{div} \mathbf{v}) - \tau \left(\nabla p_t - 2\mu_1 \Delta \mathbf{v}_t - (\lambda_1 + \mu_1) \nabla (\operatorname{div} \mathbf{v})_t \right)$$
(54)

4.3.1 Small relaxation time

For small values of τ , the stress can be represented in the form of an asymptotic expansion

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_0 + \tau \boldsymbol{\sigma}_1 + \tau^2 \boldsymbol{\sigma}_2 + \dots$$
 (55)

In zero approximation, the classical constitutive relation holds

$$\boldsymbol{\sigma}_0 = -p\mathbf{I} + 2\mu\mathbf{D} + \lambda(\mathrm{tr}\mathbf{D})\mathbf{I}.$$
(56)

The first approximation determines

$$\boldsymbol{\sigma}_1 = 2(\mu_1 - \mu)\mathbf{D}_t + (\lambda_1 - \lambda)\mathrm{tr}(\mathbf{D})_t \mathbf{I}.$$
(57)

The corresponding divergences read

$$\operatorname{div} \boldsymbol{\sigma}_0 = -\nabla p + \mu \Delta \mathbf{v} + (\lambda + \mu) \nabla(\operatorname{div} \mathbf{v}), \tag{58}$$

$$\operatorname{div} \boldsymbol{\sigma}_1 = (\mu_1 - \mu) \Delta \mathbf{v}_t + (\lambda_1 - \lambda + \mu_1 - \mu) \nabla (\operatorname{div} \mathbf{v}_t).$$
(59)

4.3.2 Incompressible fluid

As a simple example, we consider the case of incompressible fluids. The incompressibility condition

$$\operatorname{div} \mathbf{v} = 0, \tag{60}$$

reduces the relationships for divergences to

$$\operatorname{div}\boldsymbol{\sigma}_0 = -\nabla p + \mu \Delta \mathbf{v},\tag{61}$$

and, keeping the order of approximation,

div
$$\boldsymbol{\sigma}_1 = (\mu_1 - \mu)\Delta \mathbf{v}_t = (\mu_1 - \mu)\Delta \left(\frac{1}{\rho}(-\nabla p + \mu\Delta \mathbf{v})\right).$$
 (62)

Appeared equation of motion

$$\rho \mathbf{v}_t = -\nabla p + \mu \Delta \mathbf{v} + \tau (\mu_1 - \mu) \Delta \left(\frac{1}{\rho} (-\nabla p + \mu \Delta \mathbf{v}) \right), \tag{63}$$

can be compared with the gradient model by Aifantis [65]

$$\rho \mathbf{v}_t = -\nabla p + \mu (\Delta \mathbf{v} - l^2 \Delta^2 \mathbf{v}), \tag{64}$$

and the hyperstress model [66]

$$\rho \mathbf{v}_t = -\nabla p + \mu \Delta \mathbf{v} - \zeta \Delta \Delta \mathbf{v}. \tag{65}$$

Again, the internal variable approach results in a more sophisticated equation of motion.

The obtained extended models of fluid motion are thermodynamically consistent because they follow from the solution of the dissipation inequality. As usual, the internal variable is introduced to take into account the influence of motions at a microscale which cannot be accounted for explicitly.

However, the possibilities of internal variables are not exhausted yet.

5 Dual internal variables

The dual internal variable approach is the generalization of the single internal variable theory [33–35]. In the framework of this concept, it is supposed that the free energy density depends on internal variables α, β , and their space gradients

$$\psi = \psi(\rho, \theta, \alpha, \nabla \alpha, \beta, \nabla \beta).$$
(66)

Correspondingly, the equations of state are given by

$$\eta = -\frac{\partial\psi}{\partial\theta}, \quad \mathbf{A} := -\frac{\partial\psi}{\partial\alpha}, \quad \mathcal{A} := -\frac{\partial\psi}{\partial\nabla\alpha}, \quad \mathbf{B} := -\frac{\partial\psi}{\partial\beta}, \quad \mathcal{B} := -\frac{\partial\psi}{\partial\nabla\beta}, \quad (67)$$

with additional conjugate quantities \mathbf{B} and \mathcal{B} .

The Clausius-Duhem inequality keeps its form (??)

$$-\rho\psi_t - \rho\eta\theta_t - \left(\frac{\mathbf{q}}{\theta} + \mathbf{K}\right) \cdot \nabla\theta + \boldsymbol{\sigma} : \mathbf{D} + \operatorname{div}(\theta\mathbf{K}) \ge 0.$$
(68)

The time derivative of the free energy is calculated then using of the functional dependence of the free energy (66) and equations of state (67)

$$\psi_t = \frac{\partial \psi}{\partial \rho} \rho_t + \frac{\partial \psi}{\partial \theta} \theta_t + \frac{\partial \psi}{\partial \alpha} \alpha_t + \frac{\partial \psi}{\partial \nabla \alpha} \nabla \alpha_t + \frac{\partial \psi}{\partial \beta} \beta_t + \frac{\partial \psi}{\partial \nabla \beta} \nabla \beta_t.$$
(69)

Accordingly, the dissipation inequality reads

$$-\rho \frac{\partial \psi}{\partial \rho} \rho_t + \boldsymbol{\sigma} : \mathbf{D} + (\mathbf{A} - \operatorname{div} \mathcal{A}) : \boldsymbol{\alpha}_t + (\mathbf{B} - \operatorname{div} \mathcal{B}) : \boldsymbol{\beta}_t + \operatorname{div} (\mathcal{A} : \boldsymbol{\alpha}_t + \mathcal{B} : \boldsymbol{\beta}_t + \theta \mathbf{K}) - \left(\frac{\mathbf{q}}{\theta} + \mathbf{K}\right) \cdot \nabla \theta \ge 0.$$
(70)

As before, we eliminate the divergence term in the dissipation inequality following Maugin [67]

$$\mathbf{K} = -\theta^{-1}(\boldsymbol{\mathcal{A}} : \boldsymbol{\alpha}_t + \boldsymbol{\mathcal{B}} : \boldsymbol{\beta}_t).$$
(71)

This reduces the dissipation inequality to the sum of products of thermodynamic fluxes and forces taking into account Eq. (10)

$$(p\mathbf{I} + \boldsymbol{\sigma}) : \mathbf{D} + (\mathbf{A} - \operatorname{div}\mathcal{A}) : \boldsymbol{\alpha}_t + (\mathbf{B} - \operatorname{div}\mathcal{B}) : \boldsymbol{\beta}_t - \frac{1}{\theta} (\mathbf{q} - \mathcal{A} : \boldsymbol{\alpha}_t - \mathcal{B} : \boldsymbol{\beta}_t) \cdot \nabla \theta \ge 0.$$

$$(72)$$

As previously, the solution of dissipation inequality (72) will follow from the representation thermodynamic fluxes as linear functions of conjugated thermodynamic forces.

5.1 Isothermal case

In the isothermal case the dissipation inequality is even more simple

$$(p\mathbf{I} + \boldsymbol{\sigma}) : \mathbf{D} + (\mathbf{A} - \operatorname{div}\mathcal{A}) : \boldsymbol{\alpha}_t + (\mathbf{B} - \operatorname{div}\mathcal{B}) : \boldsymbol{\beta}_t \ge 0.$$
(73)

The linear solution of the dissipation inequality is obtained similarly to that in the case of single internal variable

$$\begin{pmatrix} p\mathbf{I} + \boldsymbol{\sigma} \\ \boldsymbol{\alpha}_t \\ \boldsymbol{\beta}_t \end{pmatrix} = \mathbf{L} \begin{pmatrix} \mathbf{D} \\ (\mathbf{A} - \operatorname{div}\mathcal{A}) \\ (\mathbf{B} - \operatorname{div}\mathcal{B}) \end{pmatrix},$$
(74)

where

$$\mathbf{L} = \begin{pmatrix} L_{11} & L_{12} & L_{13} \\ L_{21} & L_{22} & L_{23} \\ L_{31} & L_{32} & L_{33} \end{pmatrix},$$
(75)

with the same condition of the positive semidefiniteness of the matrix \mathbf{L} as for single internal variable case. It follows that the constitutive relation for the stress is represented as

$$p\mathbf{I} + \boldsymbol{\sigma} = L_{11}\mathbf{D} + L_{12}(\mathbf{A} - \operatorname{div}\mathcal{A}) + L_{13}(\mathbf{B} - \operatorname{div}\mathcal{B}).$$
(76)

Evolution equations for internal variables α and β have the form

$$\boldsymbol{\alpha}_t = L_{21}\mathbf{D} + L_{22}(\mathbf{A} - \operatorname{div}\mathcal{A}) + L_{23}(\mathbf{B} - \operatorname{div}\mathcal{B}), \tag{77}$$

$$\boldsymbol{\beta}_t = L_{31}\mathbf{D} + L_{32}(\mathbf{A} - \operatorname{div}\mathcal{A}) + L_{33}(\mathbf{B} - \operatorname{div}\mathcal{B}).$$
(78)

The evolution equations are coupled with one another as well as with the constitutive relation (76). Equations (77) and (78) indicate the duality between the internal variables α and β .

5.2 Quadratic free energy

In the case of a quadratic dependence of the free energy density on internal variables and their gradients

$$\psi(\dots, \boldsymbol{\alpha}, \nabla \boldsymbol{\alpha}, \boldsymbol{\beta}, \nabla \boldsymbol{\beta}) = \dots + \frac{B}{2}\boldsymbol{\alpha}^2 + \frac{C}{2}(\nabla \boldsymbol{\alpha})^2 + \frac{D}{2}\boldsymbol{\beta}^2 + \frac{F}{2}(\nabla \boldsymbol{\beta})^2, \quad (79)$$

contributions of internal variables to evolution equations can be represented as

$$\mathbf{A} - \operatorname{div} \mathcal{A} = -B\boldsymbol{\alpha} + C\Delta\boldsymbol{\alpha}, \quad \mathbf{B} - \operatorname{div} \mathcal{B} = -D\boldsymbol{\beta} + F\Delta\boldsymbol{\beta}.$$
(80)

One of the dual internal variables can be eliminated. Due to symmetry, we can choose the elimination of β . To do this, we make time differentiation of Eq. (77)

$$\boldsymbol{\alpha}_{tt} = L_{21}\mathbf{D}_t + L_{22}(-B\boldsymbol{\alpha}_t + C\Delta\boldsymbol{\alpha}_t) + L_{23}(-D\boldsymbol{\beta}_t + F\Delta\boldsymbol{\beta}_t), \quad (81)$$

and then write expressions for β_t and $\Delta\beta_t$ in terms of α using the relation

$$L_{23}(-D\beta + F\Delta\beta) = \alpha_t - L_{21}\mathbf{D} - L_{22}(-B\alpha + C\Delta\alpha), \qquad (82)$$

which follows from Eq. (77). We will have

$$\beta_{t} = L_{31}\mathbf{D} + \frac{L_{32}L_{23} - L_{22}L_{33}}{L_{23}}(-B\alpha + C\Delta\alpha) + \frac{L_{33}}{L_{23}}(\alpha_{t} - L_{21}\mathbf{D}), \quad (83)$$
$$\Delta\beta_{t} = L_{31}\Delta\mathbf{D} + \frac{L_{32}L_{23} - L_{22}L_{33}}{L_{23}}(-B\Delta\alpha + C\Delta\Delta\alpha) + \frac{L_{33}}{L_{23}}(\Delta\alpha_{t} - L_{21}\Delta\mathbf{D}). \quad (84)$$

Substituting equalities (83) and (84) into Eq. (81), we obtain the evolution equation of the internal variable α in its own terms

$$\alpha_{tt} = L_{21}\mathbf{D}_t + L_{22}(-B\alpha_t + C\Delta\alpha_t) - D(L_{31}L_{23}\mathbf{D} + (L_{32}L_{23} - L_{22}L_{33})(-B\alpha + C\Delta\alpha)) - DL_{33}(\alpha_t - L_{21}\mathbf{D}) + F(L_{31}L_{23}\Delta\mathbf{D} + (L_{32}L_{23} - L_{22}L_{33})(-B\Delta\alpha + C\Delta\Delta\alpha)) + FL_{33}(\Delta\alpha_t - L_{21}\Delta\mathbf{D}).$$
(85)

Constitutive relation (76) can be also rewritten using the internal variable α only

$$p\mathbf{I} + \boldsymbol{\sigma} = L_{11}\mathbf{D} + L_{12}(-B\boldsymbol{\alpha} + C\Delta\boldsymbol{\alpha}) + \frac{L_{13}}{L_{23}}(\boldsymbol{\alpha}_t - L_{21}\mathbf{D} - L_{22}(-B\boldsymbol{\alpha} + C\Delta\boldsymbol{\alpha})).$$
(86)

The last equation can be resolved for α_t

$$\boldsymbol{\alpha}_{t} = \frac{L_{23}}{L_{13}} (p\mathbf{I} + \boldsymbol{\sigma}) - \frac{(L_{11}L_{23} - L_{13}L_{21})}{L_{13}} \mathbf{D} - \frac{(L_{12}L_{23} - L_{13}L_{22})}{L_{13}} (-B\boldsymbol{\alpha} + C\Delta\boldsymbol{\alpha}),$$
(87)

which provides another expression for the evolution equation of the internal variable α

$$\boldsymbol{\alpha}_{tt} = \frac{L_{23}}{L_{13}} (p\mathbf{I} + \boldsymbol{\sigma})_t - \frac{(L_{11}L_{23} - L_{13}L_{21})}{L_{13}} \mathbf{D}_t - \frac{(L_{12}L_{23} - L_{13}L_{22})}{L_{13}} (-B\boldsymbol{\alpha}_t + C\Delta\boldsymbol{\alpha}_t)$$
(88)

Comparing Eqs. (85) and (88), we arrive at the solution of the dissipation inequality in the form

$$(p\mathbf{I} + \boldsymbol{\sigma})_{t} - L_{11}\mathbf{D}_{t} - L_{12}(-B\boldsymbol{\alpha}_{t} + C\Delta\boldsymbol{\alpha}_{t}) = -D(L_{13}L_{31}\mathbf{D} + L_{32}L_{13}(-B\boldsymbol{\alpha} + C\Delta\boldsymbol{\alpha})) - -DL_{33}((p\mathbf{I} + \boldsymbol{\sigma}) - L_{11}\mathbf{D} - L_{12}(-B\boldsymbol{\alpha} + C\Delta\boldsymbol{\alpha})) + F(L_{13}L_{31}\Delta\mathbf{D} + L_{32}L_{13}(-B\Delta\boldsymbol{\alpha} + C\Delta\Delta\boldsymbol{\alpha})) + FL_{33}((\Delta p\mathbf{I} + \Delta\boldsymbol{\sigma}) - L_{11}\Delta\mathbf{D} - L_{12}(-B\Delta\boldsymbol{\alpha} + C\Delta\Delta\boldsymbol{\alpha})).$$
(89)

Equations (85) and (89) constitute the most general evolution equation for the internal variable α and the constitutive relation for fluid flow in the dual internal variable approach.

5.3 Simplifications

The obtained relationships are too complicated and need to be simplified. The first step in the simplification is to eliminate higher-order space derivatives by the choice C = 0, which means, as in the case of the single internal variable, the independence of the free energy density of the gradient of the internal variable α

$$(p\mathbf{I} + \boldsymbol{\sigma})_{t} - L_{11}\mathbf{D}_{t} - L_{12}(-B\boldsymbol{\alpha}_{t}) = -D(L_{13}L_{31}\mathbf{D} + L_{32}L_{13}(-B\boldsymbol{\alpha})) - -DL_{33}((p\mathbf{I} + \boldsymbol{\sigma}) - L_{11}\mathbf{D} - L_{12}(-B\boldsymbol{\alpha})) + F(L_{13}L_{31}\Delta\mathbf{D} + L_{32}L_{13}(-B\Delta\boldsymbol{\alpha})) + FL_{33}((\Delta p\mathbf{I} + \Delta\boldsymbol{\sigma}) - L_{11}\Delta\mathbf{D} - L_{12}(-B\Delta\boldsymbol{\alpha})).$$
(90)

Accordingly, evolution equation for the internal variable α (85) reads

$$\boldsymbol{\alpha}_{tt} = L_{21}\mathbf{D}_t + L_{22}(-B\boldsymbol{\alpha}_t) - D(L_{31}L_{23}\mathbf{D} + (L_{32}L_{23} - L_{22}L_{33})(-B\boldsymbol{\alpha})) - \\ - DL_{33}(\boldsymbol{\alpha}_t - L_{21}\mathbf{D}) + F(L_{31}L_{23}\Delta\mathbf{D} + (L_{32}L_{23} - L_{22}L_{33})(-B\Delta\boldsymbol{\alpha})) + \\ + FL_{33}(\Delta\boldsymbol{\alpha}_t - L_{21}\Delta\mathbf{D}).$$
(91)

Continuing the removal of higher-order derivatives, we assume that $L_{33} = 0$ which results in

$$(p\mathbf{I} + \boldsymbol{\sigma})_t - L_{11}\mathbf{D}_t - L_{12}(-B\boldsymbol{\alpha}_t) = -D(L_{13}L_{31}\mathbf{D} + L_{32}L_{13}(-B\boldsymbol{\alpha})) - F(L_{13}L_{31}\Delta\mathbf{D} + L_{32}L_{13}(-B\Delta\boldsymbol{\alpha})),$$
(92)

and, correspondingly,

$$\alpha_{tt} = L_{21}\mathbf{D}_t + L_{22}(-B\alpha_t) - D(L_{31}L_{23}\mathbf{D} + (L_{32}L_{23})(-B\alpha)) + F(L_{31}L_{23}\Delta\mathbf{D} + (L_{32}L_{23})(-B\Delta\alpha)).$$
(93)

The next step is to substitute the expression for α_t into Eq. (92) using relationship (87)

$$(p\mathbf{I} + \boldsymbol{\sigma})_{t} - L_{11}\mathbf{D}_{t} + \frac{L_{12}BL_{23}}{L_{13}}((p\mathbf{I} + \boldsymbol{\sigma}) - L_{11}\mathbf{D} + L_{12}B\boldsymbol{\alpha}) = = -L_{12}B(-L_{21}\mathbf{D} + L_{22}B\boldsymbol{\alpha}) - D(L_{13}L_{31}\mathbf{D} + L_{32}L_{13}(-B\boldsymbol{\alpha})) + F(L_{13}L_{31}\Delta\mathbf{D} + L_{32}L_{13}(-B\Delta\boldsymbol{\alpha})).$$
(94)

A big amount of coefficients impedes the analysis but provides a lot of possibilities for modeling. As an example let us consider the situation characterizing by values D = 0 and $BL_{12} = 1$. Constitutive relation (94) reduces to

$$(p\mathbf{I} + \boldsymbol{\sigma})_t - L_{11}\mathbf{D}_t + \frac{L_{23}}{L_{13}}\left((p\mathbf{I} + \boldsymbol{\sigma}) - L_{11}\mathbf{D} + \boldsymbol{\alpha}\right) - (-L_{21}\mathbf{D} + L_{22}B\boldsymbol{\alpha}) = F(L_{13}L_{31}\Delta\mathbf{D} + L_{32}L_{13}(-B\Delta\boldsymbol{\alpha})),$$
(95)

and evolution equation for the internal variable (93) reads, accordingly,

$$\alpha_{tt} = L_{21}\mathbf{D}_t + L_{22}(-B\alpha_t) + F(L_{31}L_{23}\Delta\mathbf{D} + (L_{32}L_{23})(-B\Delta\alpha)).$$
(96)

Denoting $L_{13} = \tau$ we rearrange constitutive relation (95) to the form

$$\tau(p\mathbf{I} + \boldsymbol{\sigma})_t - \tau L_{11}\mathbf{D}_t + L_{23}\left((p\mathbf{I} + \boldsymbol{\sigma}) - L_{11}\mathbf{D} + \boldsymbol{\alpha}\right) + \tau \left(L_{21}\mathbf{D} - L_{22}B\boldsymbol{\alpha}\right) = F\tau^2 (L_{31}\Delta\mathbf{D} - L_{32}(B\Delta\boldsymbol{\alpha})).$$
(97)

It is clear that for small values of τ we have almost classical constitutive relation, but with the contribution of the internal variable

$$(p\mathbf{I} + \boldsymbol{\sigma}) - L_{11}\mathbf{D} + \boldsymbol{\alpha} = \mathbf{0}.$$
 (98)

In the absence of internal variables it reduces to the classical case.

5.4 Equations of motion

As in the case of the single internal variable, the divergence of σ follows from Eq. (97)

$$\tau(\nabla p + \operatorname{div} \boldsymbol{\sigma})_t - \tau L_{11} \Delta \mathbf{v}_t + L_{23} \left((\nabla p + \operatorname{div} \boldsymbol{\sigma}) - L_{11} \Delta \mathbf{v} + \operatorname{div} \boldsymbol{\alpha} \right) + \tau \left(L_{21} \Delta \mathbf{v} - L_{22} B \operatorname{div} \boldsymbol{\alpha} \right) = F \tau^2 (L_{31} \Delta \operatorname{div} \mathbf{v} - L_{32} (B \Delta \operatorname{div} \boldsymbol{\alpha})).$$
(99)

Substituting the divergence into the balance of linear momentum, we arrive at

$$\rho \mathbf{v}_t + \frac{\tau}{L_{23}} \rho \mathbf{v}_{tt} = -\nabla p + L_{11} \Delta \mathbf{v} - \operatorname{div} \boldsymbol{\alpha} - \frac{\tau}{L_{23}} (\nabla p)_t + \frac{\tau L_{11}}{L_{23}} \Delta \mathbf{v}_t - \frac{\tau}{L_{23}} (L_{21} \Delta \mathbf{v} - L_{22} B \operatorname{div} \boldsymbol{\alpha}) + F \frac{\tau^2}{L_{23}} (L_{31} \Delta \operatorname{div} \mathbf{v} - L_{32} (B \Delta \operatorname{div} \boldsymbol{\alpha})).$$
(100)

As one can see, there exist different modes of flow depending on the value of τ . If τ is small, a fluid motion (at least in the first approximation) is governed by

$$\rho \mathbf{v}_t = -\nabla p + L_{11} \Delta \mathbf{v} - \operatorname{div} \boldsymbol{\alpha}. \tag{101}$$

This equation looks similarly to the Navier–Stokes equation of motion. However, the last term in the right hand side depends on the divergence of the internal variable α , whose evolution is determined by Eq. (96) which is a hyperbolic equation if coefficients L_{32} and L_{23} have alternate signs.

For big values of τ , the fluid motion satisfies a hyperbolic equation (for negative values of L_{21})

$$\rho \mathbf{v}_{tt} = -(\nabla p)_t + L_{11} \Delta \mathbf{v}_t - (L_{21} \Delta \mathbf{v} - L_{22} B \operatorname{div} \boldsymbol{\alpha}) + F \tau (L_{31} \Delta \operatorname{div} \mathbf{v} - L_{32} (B \Delta \operatorname{div} \boldsymbol{\alpha}))$$
(102)

To keep the same order of value for all terms, it is convenient to set $F = 1/\tau$. The evolution equation for the internal variable α is still hyperbolic equation (96). As before, any invariant material time derivative can be used in equations of motion.

6 Conclusions

The internal variables theory provides a framework for accounting the influence of processes at a microscale which cannot be described explicitly. Based on the exploitation of the Clausius–Duhem inequality, the internal variable theory produce the extension of the Navier–Stokes equations even in the case of the linear solution of the dissipation inequality for isothermal situation. Remarkable is that the single internal variable can be eliminated from the consideration if the dependence of the free energy density on the internal variable is quadratic. Obtained constitutive relations and equations of motion confirm the thermodynamic consistency of existing Maxwell-type models.

The dual internal variables concept provides new possibilities to formulate more complicated models of fluid motion. An essential part of the theory is the hyperbolic evolution equation for the internal variable, which is coupled with the equation of motion. An intriguing feature of the extended model is the opportunity to distinguish two specific modes of flow depending on values of coefficients. It is difficult to say that these two types of flow can be associated with laminar and turbulent motion. However, there are so many aspects of turbulent flows [68, e.g.] that various models can be valid in specific cases.

The alternative approach to take the effect of a microstructure into account [69, 70] is based on the concept of morphological descriptors [71]. This notion is more general than the internal variable one. However, the evolution equations for the descriptors follow from variational principles and, therefore, they are applicable to conservative systems. Dissipative effects (like viscosity) are introduced additionally and need special consideration.

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