Entropy production equation

We assume the existence of specific entropy \( \eta \) as a function of the state variables (e.g., \( \eta = \tilde{\eta}(e, \varrho) \)) and assume that it satisfies the following properties:

- \( \eta \) is an increasing function with respect to \( e \) and the absolute temperature is given by 
  \[
  \theta = \text{def} \, \frac{1}{\varrho \eta'}, \quad \eta' = \frac{d\eta}{de} \geq 0.
  \]
- \( \eta \to 0^+ \) as \( \theta \to 0^+ \) (Nernst postulate).
- \( S(t) = \text{def} \int_{\Omega} (\varrho \eta)(t, \cdot) \, dx \) tends to its maximum as \( t \to \infty \) provided that the body is thermally and mechanically isolated (Entropy maximum principle).

The local form of the entropy balance is in the form

\[
\varrho \eta - \text{div} \left( \frac{\varrho}{\theta} \right) \left[ T_3 : D_3 + (m + p(\eta, \varrho)) \right] \text{div} \, v + \varrho r + \frac{\varrho \cdot \nabla \theta}{\theta} \right],
\]

where we have used

\[
p(\eta, \varrho) = \text{def} \, \varrho \theta^2 \frac{\partial e}{\partial \theta}(\eta, \varrho),
\]
\[
m = \text{def} \, \frac{1}{3} \text{Tr} \, \mathbb{T},
\]
\[
T_3 = \text{def} \, \mathbb{T} - mI.
\]

The second law of thermodynamics says that the production of entropy has to be non-negative. More explicitly, on setting

\[
\varrho \zeta = \text{def} \, \frac{1}{\theta} \left[ T_3 : D_3 + (m + p(\eta, \varrho)) \right] \text{div} \, v + \frac{\varrho \cdot \nabla \theta}{\theta} + \varrho r,
\]

or

\[
\varrho \theta \zeta = \text{def} \, T_3 : D_3 + (m + p(\eta, \varrho)) \text{div} \, v + \frac{\varrho \cdot \nabla \theta}{\theta} + \varrho r,
\]

the second law of thermodynamics implies that

\[
\xi = \text{def} \, \varrho \theta \zeta \geq 0.
\]

In [3], we identify four mechanisms leading to entropy production: the first one associated with isochoric motions as shear, the second due to volume changes, the third due to conduction of heat, and the last one due to radiation. Note that all these terms are in the form of the product of a thermodynamic affinity taken from the set \( \{ D_3, \text{div} \, v, \nabla \theta, \varrho \} \) and a corresponding thermodynamical flux taken from the set \( \{ T_3, (m + p(\eta, \varrho)), q(\theta, r) \} \). It is important to notice that variations of fluxes cause changes in affinities, and not the other way around. This point cannot be overemphasized if we were to turn causality upside down. It is forces (stresses) that cause deformation (and hence velocity gradients) and not vice-versa.

Let \( \psi \) denote the specific Helmholtz free energy and \( \xi \) the rate of dissipation associated with the material. In an isothermal process with no radiation, the rate of dissipation \( \xi \) is given by the energy-dissipation equation (reduced thermodynamical inequality)

\[
T : D - \varrho \dot{\psi} = \xi \geq 0,
\]

where \( T : D \) is usually referred to as the stress power.

We shall make constitutive assumptions for the Helmholtz free energy \( \psi \) and rate of dissipation \( \xi \). We assume

\[
\psi = \tilde{\psi} \left( \text{Tr} \, B_{\kappa_{p(t)}} \, \text{Tr} \, B_{\kappa_{p(t)}}^2 \right),
\]

which is tantamount to the instantaneous elastic response between \( \kappa_{p(t)}(B) \) and \( \kappa_{i}(B) \) being that for an incompressible material that is isotropic with respect to \( \kappa_{p(t)} \). For the rate of dissipation, we assume

\[
\xi = \tilde{\xi} \left( B_{\kappa_{p(t)}}, D_{\kappa_{p(t)}} \right),
\]

where we also stipulate \( \tilde{\xi}(\cdot, 0) = 0 \).

The response of a neo-Hookean material is

\[
\varrho \dot{\psi} = \frac{\nu}{2} \left( \text{Tr} \, B_{\kappa_{p(t)}} - 3 \right) \Rightarrow \varrho \dot{\psi} = \nu B_{\kappa_{p(t)}} : D - \nu F_{\kappa_{p(t)}} D_{\kappa_{p(t)}} : F_{\kappa_{p(t)}}
\]

where the material constant \( \nu \) represents the elastic modulus.
**Classical models**

**Classical upper convected Maxwell fluid**

\[ T = -pI + S, \]
\[ S + \tau \dot{S} = 2\mu \mathbb{D}, \]

where \( \tau \) is a *relaxation time* saying how fast the stress decreases in the stress relaxation test and \( \mu \) is the viscosity.

**Oldroyd-B model**

\[ T = -pI + S, \]
\[ S + \lambda_1 \dot{S} = \mu \left( \mathbb{D} + \lambda_2 \mathbb{D} \right), \]

where \( \mu \) is the viscosity and \( \lambda_1 \) and \( \lambda_2 \) are the *relaxation* and *retardation* times. This model behaves more visously than the Maxwell model.

*Remark.* This model can be also rewritten in the form

\[ T = -pI + 2\mu \mathbb{D} + S, \]
\[ S + \tau \dot{S} = 2\mu_1 \mathbb{D}, \]

*Remark.*

\[ \tilde{\rho} \tilde{\psi} = \frac{\nu}{2} \left( \text{Tr} \mathbb{B}_{\kappa_\text{ref}(t)} - 3 - \ln \det \mathbb{B}_{\kappa_\text{ref}(t)} \right) \]

**Isotropic homogeneous compressible Cauchy elastic solid**

\[ T = \lambda_0 I + \lambda_1 \mathbb{B} + \lambda_2 \mathbb{B}^2, \]

where \( \lambda_i, i = 0, 1, 2 \) are functions of \( \text{Tr} \mathbb{B}, \frac{1}{2} \left( (\text{Tr} \mathbb{B})^2 - \text{Tr} \mathbb{B}^2 \right) \) and \( \det \mathbb{B} \).

**Hyperelastic material**

Truesdell introduced the notion of *hypo-elasticity* as a possible model for the non-linear behavior of solids that reduces appropriately to the classical approximation of linearized elasticity.

According to Truesdell, the stress in a hypo-elastic material is given by

\[ T = \tilde{g}(T, L) \]

From eq. (8) and the assumptions \( \psi = \psi(F) \), we obtain

\[ T : D - \rho \frac{\partial \tilde{\psi}}{\partial F} : \mathbb{F} = T : L - \rho \frac{\partial \tilde{\psi}}{\partial F} : \mathbb{F} = \left( T - \rho \frac{\partial \tilde{\psi}}{\partial F} F^T \right) : L, \]

implying\(^1\)

\[ T = \rho \frac{\partial \tilde{\psi}}{\partial F} F^T, \]

which is an alternative definition of hyperelastic material, see Kružík & Roubíček.

It might be convenient to work with the *Piola-Kirchhoff stress* \( T =\text{det}(\text{det} F) F^{-1} \mathbb{F}^{-T} \), and introduce the dissipation equation (8) as

\[ T_R : \dot{\mathbb{F}} - \rho_{\text{ref}} \tilde{\psi} = \xi \geq 0, \]

where \( \rho_{\text{ref}} \) denotes the reference density. Then, for \( \psi = \tilde{\psi}(E) \), we obtain

\[ T_R = \rho_{\text{ref}} \frac{\partial \tilde{\psi}}{\partial E} \]

which is equivalent to eq. (18).

**Constitutive equations for the rate of dissipation**

**Classical incompressible Navier-Stokes fluid with constant viscosity**

\[ \dot{\xi} = 2\mu |D|^2 = 2\mu |D_\delta|^2 \]

\(^1\)If the body is incompressible, then \( T = \Phi I + \rho \frac{\partial \tilde{\psi}}{\partial F} F^T \).
Classical compressible Navier-Stokes fluid

\[ \dot{\xi} = 2\mu(\rho)|D|^2 + \lambda(\rho)(\text{div } v)^2 = \frac{2\mu(\rho) + 3\lambda(\rho)}{2}(\text{div } v)^2 \]  

(22)

In order to fulfill (7), one requires that

\[ \mu(\rho) \geq 0 \quad \text{and} \quad 2\mu(\rho) + 3\lambda(\rho) \geq 0. \]  

(23)

It is sometimes said that the ideal fluid (meaning the fluid that does not dissipate energy) is inviscid if

\[ \mu(\rho) = \lambda(\rho) = 0. \]

In no real fluid are the viscosities zero. However, it is possible in certain flows that the deviatoric part of the Cauchy stress is absent (i.e., \( T_\delta = 0 \)) and the stress is essentially spherical.

This leads to an alternative entropy production formulation

\[ \dot{\xi} = \frac{1}{2\mu(\rho)}|T_\delta|^2 + \frac{3}{2\mu(\rho) + 3\lambda(\rho)}(m + p(\rho))^2, \]  

(24)

that fulfills the second law of thermodynamics (7) if

\[ \mu(\rho) > 0 \quad \text{and} \quad 2\mu(\rho) + 3\lambda(\rho) > 0. \]

(25)

Note that it follows from (24), (25) that

\[ \xi = 0 \iff T_\delta = 0 \quad \text{and} \quad m = -p(\rho), \]  

(26)

implying that

\[ T = -p(\rho)\mathbb{1}, \]  

(27)

which is the constitutive relation for the Euler (or elastic) fluid.

Incompressible fluid with shear, density and pressure dependent viscosity

\[ \dot{\xi} = 2\mu(\rho,p,|D|)|D|^2 = 2\mu(\rho,p,|D|)|D_\delta|^2 \]

(28)

\[ p = -\frac{1}{\beta} \text{Tr } T. \]

Incompressible power-law like viscoelastic model

\[ \dot{\xi} = \varepsilon_1 \left( \varepsilon_0 + |D|^2 \right)^{\alpha-1} |D|^2 + \varepsilon_2 \left( D_{\kappa p(i)} : C_{\kappa p(j)} D_{\kappa p(j)} \right)^2 \]

(29)

for \( \varepsilon_0, \varepsilon_1, \varepsilon_2 > 0, \alpha \in \mathbb{R}, \beta > 0.5. \)

Compressible fluid with shear, density and pressure dependent viscosity, Málek and Rajagopal (2010)

\[ \dot{\xi} = \xi(\rho, m + p(\rho), \text{div } v, T_\delta, D_\delta) \geq 0 \]

(30)

and in the case of zero thermodynamical fluxes,

\[ \dot{\xi}(\rho, 0, \text{div } v, 0, D_\delta) = 0. \]

Examples of compressible power-law fluids (in the form of eq. (24)):

- \( \mu = \mu(\rho, \text{div } v, |D_\delta|^2) \), \( \lambda = \lambda(\rho, \text{div } v) \) \( \implies \) both shear and bulk viscosity depend on \( \text{div } v \) and the generalized shear rate \( |D_\delta|^2 \).
- \( \mu = \mu_* \), \( \lambda(\rho, \text{div } v) \) \( \implies \) shear viscosity is constant and the bulk viscosity depends on \( \text{div } v \).
- \( \mu_{\text{shear}} = \mu_{\text{shear}}(\text{div } v, |D_\delta|^2) \), \( \mu_{\text{bulk}} = \mu_{\text{bulk}}(\text{div } v, |D_\delta|^2) \)
- \( m = -p(\rho) \) (the fluid does not dissipate energy due to volumetric changes)
  - \( \mu = \mu(|D_\delta|) = \mu_* |D_\delta|^{-2} \), \( r \leq 2 \)
    \[ \dot{\xi} = \frac{|T_\delta|^2}{2\mu_* |D_\delta|^{-2}} \implies T_\delta = 2\mu_* |D_\delta|^{-2} D_\delta \]
  - \( r > 2 \) \( \implies \) shear thickening fluid, \( r < 2 \) \( \implies \) shear thinning fluid
  - \( \mu = \mu(|T_\delta|) = \frac{1}{r} (2\mu_*)^{\frac{r}{r-2}} |T_\delta|^{\frac{2}{r-2}} \), \( r \in (1, \infty) \)
    \[ \dot{\xi} = \left( \frac{1}{2\mu_*} \right)^{\frac{1}{r-2}} |T_\delta|^{\frac{r}{r-2}} \implies D_\delta = \left( \frac{1}{2\mu_*} \right)^{\frac{1}{r-2}} |T_\delta|^{\frac{r}{r-2}} T_\delta \]
Compressible Bingham fluid, Málek and Rajagopal (2010)

\[ \dot{\xi} = \frac{|D_\delta| |T_\delta|^2}{\tau_0}, \]

where \( \tau_0 > 0 \) represents the threshold (yield stress), we arrive at

\[ D_\delta = |D_\delta| \frac{T_\delta}{\tau_0}, \]

from which follows that

- If \( |T_\delta| < \tau_0 \) then \( D_\delta \equiv 0 \),
- If \( |T_\delta| = \tau_0 \) then \( \frac{D_\delta}{|D_\delta|} = \frac{T_\delta}{\tau_0} \) for \( D_\delta \neq 0 \).

Compressible viscous Bingham and Herschel-Bulkley fluids (Case II), Málek and Rajagopal (2010)

\[ \dot{\xi} = \frac{1}{2\mu (|D_\delta|^2)} f \left( \left( |T_\delta| - \tau_0 \right)^+ |T_\delta|^2 = \text{def} \frac{1}{2\mu (|D_\delta|^2)} \left( \left( |T_\delta| - \tau_0 \right)^+ |T_\delta|^2 \right) \right) \]

where again \( \tau_0 > 0 \) represents the threshold (the yield stress), we obtain

\[ 2\mu \left( |D_\delta|^2 \right) D_\delta = f \left( \left( |T_\delta| - \tau_0 \right)^+ \right) T_\delta, \]

from which follows that

- If \( |T_\delta| \leq \tau_0 \) then \( \tau_\delta \equiv 0 \),
- If \( |T_\delta| > \tau_0 \) then \( \tau_\delta = 2\mu \left( |D_\delta|^2 \right) f \left( \left( |T_\delta| - \tau_0 \right)^+ \right) D_\delta. \)

General incompressible setting, Málek and Rajagopal (2007)

\[ \dot{\xi} = \bar{\xi} \left( \rho, p, D_\delta, D_{\kappa_{p(t)}} \right) = \mu \left( \rho, p, \gamma \right) \gamma, \quad \gamma = \varepsilon_0 |D|^2 + \varepsilon_1 D_{\kappa_{p(t)}} : C_{\kappa_{p(t)}} D_{\kappa_{p(t)}} \]

It clearly follows from \( C_{\kappa_{p(t)}} = \text{def} F_{\kappa_{p(t)}}^T F_{\kappa_{p(t)}} \) that \( \xi \geq 0 \) provided that \( \mu = \mu \left( \rho, p, \gamma \right) \) and \( \varepsilon_0 \geq 0, \varepsilon_1 \geq 0 \).

- When \( \varepsilon_1 \rightarrow 0 \), it can be shown that \( \nu = 0 \) in eq. (11) and we obtain the classical incompressible fluid model with nonconstant viscosity, not being capable of capturing phenomena such as stress relaxation, nonlinear creep, etc.
- When \( \varepsilon_0 > 0 \), we obtain Oldroyd type fluid model.
- Letting \( \varepsilon_0 \rightarrow 0 \), we obtain Maxwell type fluid model.
- If \( \mu = \mu_0 \) and the density in the reference configuration is uniform (i.e., \( \rho = \rho_0 > 0 \)) we obtain a slight modification of the model originally derived in Rajagopal and Srinivasan (2000).

Maxwell-like model, Rajagopal and Srinivasan (2000)

\[ \dot{\xi} = \mu D_{\kappa_{p(t)}} : B_{\kappa_{p(t)}} D_{\kappa_{p(t)}} \]

- Purely viscous behaviour – shear modulus \( \nu = 0 \) in eq. (11) tends to infinity while \( \mu \) is finite and we recover the constitutive equation for a Newtonian viscous fluid.
- Purely elastic behavior – ‘viscosity’ \( \mu \) tends to infinity while \( \nu \) in eq. (11) is finite and we recover the constitutive equation for a neo-Hookean solid.
- Relationship to the upper convected Maxwell model – the main difference is that while the material modulus \( \left( \frac{\mu}{\tau} \right) \) in eq. (12) is a constant, the material modulus \( \Lambda \) is a function of the elastic stretch.

\[ T = -p I + \Sigma, \]

\[ \Sigma + \left( \frac{\mu}{2\nu} \right) \frac{\partial}{\partial t} \frac{\partial}{\partial \nu} = \lambda \left( B_{\kappa_{p(t)}} \right) I \]

4
If the elastic strain is small in the sense that
\[ \| B_{\kappa(\tau)} - I \| = O(\epsilon), \quad \epsilon \ll 1, \]
the model reduces to the classical upper convected Maxwell model. In other words, the upper convected Maxwell model can be viewed as a linearized elastic response from an evolving class of natural configurations, the evolution being determined by the rate of dissipation of the form (36).

Remark (Variant of the Maxwell-like model).
\[ \hat{\xi} = \mu D_{\kappa(\tau)} : D_{\kappa(\tau)} \] (37)

This model has a different ‘relaxation parameter’. For small elastic strains, it also reduces to the upper-convected Maxwell model.

Oldroyd-B type model, Rajagopal and Srinivasa (2000)

Added an extra dissipative term mimicking that for a Newtonian fluid to the form (36)
\[ \hat{\xi} = \mu D_{\kappa(\tau)} : D_{\kappa(\tau)} + \mu_1 D : D \] (38)

Assuming that the elastic strain is small, the model reduces to that of the Oldroyd-B fluid.

Objective time derivatives

The time derivative can be chosen from the family of *Gordon-Schowalter objective time derivatives* given by
\[ \frac{\delta A}{\delta t}_a = \text{def} \frac{\partial A}{\partial t} + (v \cdot \nabla) A - (WA - AW) + a (DA + AD), \quad a \in [-1, 1]. \] (39)

- \( a = -1 \) (upper convected Oldroyd derivative)
  \[ \overset{\circ}{A} = \text{def} \frac{\partial A}{\partial t} + (v \cdot \nabla) A - \mathbb{I} A - A \mathbb{I}^T \]

- \( a = 0 \) (co-rotational (Jaumann) derivative)
  \[ \overset{\text{o}}{A} = \text{def} \frac{\partial A}{\partial t} + (v \cdot \nabla) A - WA + AW \]

- \( a = 1 \) (lower convected Oldroyd derivative)
  \[ \overset{\circ}{A} = \text{def} \frac{\partial A}{\partial t} + (v \cdot \nabla) A + A \mathbb{L} + \mathbb{L}^T A \]

References


