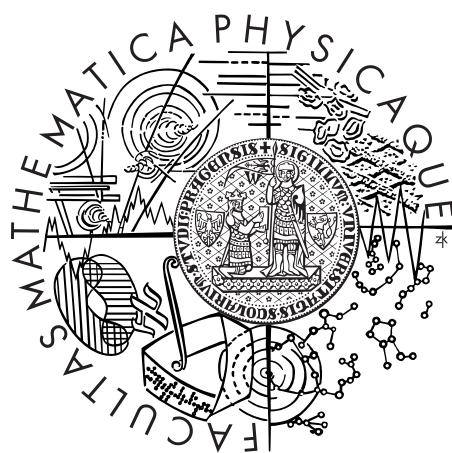# Mechanics and thermodynamics of viscoelastic fluids

Habilitation thesis

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Mechanics and thermodynamics of viscoelastic fluids

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Contents

Thesis outline

The habilitation thesis is based on the research in **theory of viscoelastic-rate-type fluids**. Research papers [**P7**], [**P5**] and [**P6**] are focused on **physical underpinnings** and **thermodynamics** of the given mathematical models. Subsequently, the proper understanding of the physical underpinnings of the given models is exploited in papers [**P3**], [**P2**] and [**P4**] in **finite amplitude stability analysis** of flows of the fluids described by these models. The stability analysis is based on general concepts introduced in [**P1**]. Finally, papers [**P9**] and [**P10**] deal with mathematical description of certain **nonlinear phenomena** encountered in experimental investigation of viscoelastic rate-type fluids, whereas these papers use the general approach introduced in [**P8**].

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[**P10**] Řehoř, M., V. Průša, and K. Tůma. On the response of nonlinear viscoelastic materials in creep and stress relaxation experiments in the lubricated squeeze flow setting. *Phys. Fluids*, 28(10):103102, 2016. doi: 10.1063/1.4964662.

CHAPTER 1

Introduction

1. Beyond Navier–Stokes equations

Majority of works focused on mathematical modelling of fluid flows use the classical Navier–Stokes equations. The equations were gradually developed in 19th century by Navier [1823], Poisson [1831], Saint-Venant [1843] and Stokes [1845], and since then they have been successfully used to describe and explain various fluid flow phenomena especially in substances such as water and air. In particular, the advent of computers gave rise to the computational fluid dynamics, and the numerical solution of Navier–Stokes equations in complex geometries became an indispensable tool in science and technology. There are, however, fluid flow phenomena that are beyond the reach of Navier–Stokes equations.

While in the early days of Navier–Stokes equations the fluids of interest were predominantly water and air, thorough the 20th century the interest expanded to substances such as oils, molten polymers and biological fluids. For such fluids the Navier–Stokes equations cease to provide an adequate description of the corresponding fluid motion, and the whole field of *non-Newtonian fluids* emerged. The term "non-Newtonian fluids" reflects the *departure from the linear relation between the shear stress and the shear rate*. For *Newtonian* fluids—and subsequently the Navier–Stokes equations—the linear relation between the shear stress and the shear rate is assumed, and this assumption goes back to [Newton, 1687, Book II, Section IX]:

> The resistance arising from the friction [*lit.* lack of lubricity or slipperiness] of
> the parts of fluid is, other things being equal, proportional to the velocity with
> which the pars of the fluid are separated from one another[1].

For *non-Newtonian* fluids such a linear relation does not hold, and more elaborate relation between the shear stress and the shear rate—or more precisely between the Cauchy stress tensor and the symmetric part of the velocity gradient—must be used.

The first simple mathematical models for non-Newtonian fluids did not differ significantly from the classical Newtonian assumption. Instead of the linear relationship between the shear stress and shear rate, models based on shear dependent viscosity assumption were proposed, see, for example, Ostwald [1925] and de Waele [1923]. This class of models can be used, for example, to model the important shear-thinning/shear-thickening effect. However, these models fail to predict important non-Newtonian effects such as normal stress differences in simple shear flows, creep and stress relaxation and so forth, that give rise to visually stunning phenomena such as rod-climbing effect, see especially the seminal paper by Weissenberg [1947]. (For a detailed description of various non-Newtonian effects see Tanner and Walters [1998] or newer texts such as Málek and Rajagopal [2005] or Larson and Desai [2015] and references therein.) The need to model the effects that are beyond the reach of the classical Navier–Stokes equations subsequently lead to more sophisticated mathematical models.

Indeed, the research activity in the second half of 20th century lead to various competing classes of models regarding non-Newtonian fluids. The approaches to the development of mathematical models were ranging from purely phenomenological models/concepts such as Reiner–Rivlin fluid, Rivlin [1948], Rivlin–Ericksen fluid, Rivlin and Ericksen [1955], Green and Rivlin [1957], integral type models Bernstein et al. [1963], fluids with fading memory, Coleman and Noll [1960], to micro-macro models Kramers [1946]. (See Tanner and Walters [1998] for a detailed historical account and Larson [1988], Bird et al. [1987b,a], Phan-Thien [2013] and Truesdell and Noll [2004] for technical details concerning various classes of models.) Arguably, the best class of models that emerged

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[1]Quoted from English translation Newton [1999].

from this period are the *viscoelastic rate-type models* stemming from the seminal work by Oldroyd [1950].

The model developed by Oldroyd [1950] is a purely *phenomenological model*, which means that it exclusively works with *macroscopic* quantities. This implies that the models from this class are conceptually very simple in the sense that they are not based on assumptions concerning the internal structure of the given fluid, the models are calibrated by relatively simple macroscopic rheological measurements. (This could be also a drawback if one is *interested* in the internal structure and details concerning its evolution. But this is usually not the case in engineering practice focused on *flows* of macroscopic amount of fluids in complex geometries.) Furthermore, given the nature of the quantities entering the models, there are no substantial problems with the set-up of initial conditions and boundary conditions for these models, which could be an issue for other classes of models. Consequently, using this class of models it is straightforward to formulate initial–boundary value problems, and, in principle, solve these problems numerically, see Alves et al. [2021] and references therein for a state-of-the-art review on the corresponding computational issues.

To cut the long story short, the *viscoelastic rate-type models* are—with a bit of exaggeration— the second most frequently used models for fluid flows after the Navier–Stokes model. As such they deserve utmost attention, and the main obstacle in dealing with these models is their nonlinearity. Indeed, while the Navier–Stokes equations (for incompressible fluids) contain just one nonlinearity due to the material time derivative (convective term), the viscoleatic rate-type models contain multiple nonlinearities. Furthermore, the system of governing equations is more complex than that in the Navier–Stokes model—the viscoelastic rate-type models introduce new tensorial quantities that are governed by additional evolution equations.

The present thesis summarises some results concerning viscoelastic rate-type models. It consists of contributions focused on *physical underpinnings* and *thermodynamics* of the given mathematical models, applications of thermodynamics in *finite amplitude stability analysis* of corresponding fluid flows, and, finally, on mathematical issues regarding the description of *mechanical response* of these fluids.

2. Viscoelastic rate-type fluids

Before we proceed with detailed comments regarding the results, we briefly introduce the basic viscoelastic rate-type model—the Oldroyd-B model. Subsequently we point out some fundamental differences between the Navier–Stokes model and the Oldroyd-B model, and, for that matters, the differences between the Navier–Stokes model and the whole class of viscoelastic models based on seminal work by Oldroyd [1950]. In this introductory section we for the sake of simplicity focus on incompressible fluids only.

2.1. Incompressible Navier–Stokes–Fourier equations.

2.1.1. *Governing equations.* The standard Navier–Stokes model for flow of an incompressible fluid reads

$$\operatorname{div} \boldsymbol{v} = 0, \tag{1a}$$

$$\rho \frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = \operatorname{div} \mathbb{T} + \rho \boldsymbol{b}, \tag{1b}$$

where $\boldsymbol{v}$ denotes the (Eulerian) velocity field, ρ is the fluid density, $\boldsymbol{b}$ is the external body force and $\mathbb{T}$ is the Cauchy stress tensor. The Cauchy stress tensor is assumed to take the form

$$\mathbb{T} =_{\mathrm{def}} -p\mathbb{I} + \mathbb{T}_\delta, \tag{1c}$$

where the *traceless part* of the Cauchy stress tensor $\mathbb{T}_\delta$ is assumed to be given by the formula

$$\mathbb{T}_\delta =_{\mathrm{def}} 2\nu\mathbb{D}, \tag{1d}$$

where ν denotes the dynamic viscosity (a constant) and $\mathbb{D}$ denotes the symmetric part of the velocity gradient, $\mathbb{D} =_{\mathrm{def}} \frac{1}{2}\left(\nabla\boldsymbol{v} + (\nabla\boldsymbol{v})^\top\right)$. The symbol $\mathbb{A}_\delta$ is hereafter used for the *traceless part* (deviatoric part) of the corresponding tensor

$$\mathbb{A}_\delta =_{\mathrm{def}} \mathbb{A} - \frac{1}{3}\left(\operatorname{Tr}\mathbb{A}\right)\mathbb{I}, \tag{1e}$$

while the symbol $\frac{\mathrm{d}}{\mathrm{d}t}$ denotes the standard *material time derivative*,

$$\frac{\mathrm{d}}{\mathrm{d}t} =_{\mathrm{def}} \frac{\partial}{\partial t} + \boldsymbol{v} \bullet \nabla \tag{1f}$$

of the given Eulerian quantity. (Equation (1d) is the modern version of Newton's assumption quoted in Section 1 on page 9. Any deviation from (1d) leads to a *non-Newtonian* fluid model.) If needed, equations (1a) and (1b) can be easily completed by the evolution equation for the temperature,

$$\rho c_{\mathrm{V}} \frac{\mathrm{d}\theta}{\mathrm{d}t} = \mathrm{div}\,(\kappa \nabla \theta) + 2\nu \mathbb{D} : \mathbb{D}, \tag{1g}$$

where θ denotes the temperature, c_{V} denotes the specific heat capacity at constant volume and κ denotes the thermal conductivity. Both c_{V} and κ are assumed to be constant. (In the temperature evolution equation we use Fourier law.) The complete system of governing equations 1 is referred to as the *Navier–Stokes–Fourier* equations/model, while the fluids described by this model are referred to as the *Navier–Stokes–Fourier* fluids.

2.1.2. *Thermodynamics.* Concerning thermodynamic background of Navier–Stokes–Fourier fluids, everything is clear. The energy of such a fluid can exist in two forms—the *thermal energy* and the *kinetic energy.* It is straightforward to show that the kinetic energy is according to the model *dissipated* and converted into the thermal form, and that the term that characterises the conversion is the term $2\nu \mathbb{D} : \mathbb{D}$ in the temperature evolution equation (1g).

2.2. Oldroyd-B model.

2.2.1. *Governing equations.* The original Oldroyd-B model for flow of an incompressible fluid reads

$$\mathrm{div}\,\boldsymbol{v} = 0, \tag{2a}$$

$$\rho \frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = \mathrm{div}\,\mathbb{T} + \rho\boldsymbol{b}, \tag{2b}$$

where the Cauchy stress tensor is again given by the formula (1c), but its traceless part is given by the formula

$$\mathbb{T}_\delta =_{\mathrm{def}} 2\nu \mathbb{D} + \mu \big(\mathbb{B}_{\kappa_{p(t)}} \big)_\delta, \tag{2c}$$

where the quantity $\mathbb{B}_{\kappa_{p(t)}}$ is known to be a symmetric positive definite tensor. (Compare (2c) with the Navier–Stokes model (1d).) The evolution of the new tensorial quantity $\mathbb{B}_{\kappa_{p(t)}}$ is governed by the equation

$$\nu_1 \overline{\mathbb{B}_{\kappa_{p(t)}}}^{\nabla} + \mu \left(\mathbb{B}_{\kappa_{p(t)}} - \mathbb{I} \right) = \mathbb{0}, \tag{2d}$$

wherein ν_1 and μ are material parameters (constants). The symbol $\overset{\nabla}{\mathbb{A}}$ denotes the so-called *Oldroyd derivative* or *upper convected derivative* of the corresponding tensorial quantity $\mathbb{A}$. The upper convected derivative is defined as

$$\overset{\nabla}{\mathbb{A}} =_{\mathrm{def}} \frac{\mathrm{d}\mathbb{A}}{\mathrm{d}t} - \mathbb{L}\mathbb{A} - \mathbb{A}\mathbb{L}^{\mathsf{T}}, \tag{3}$$

where $\mathbb{L} =_{\mathrm{def}} \nabla \boldsymbol{v}$ denotes the velocity gradient and where $\frac{\mathrm{d}\mathbb{A}}{\mathrm{d}t}$ is the standard material time derivative, $\frac{\mathrm{d}\mathbb{A}}{\mathrm{d}t} =_{\mathrm{def}} \frac{\partial \mathbb{A}}{\partial t} + (\boldsymbol{v} \bullet \nabla)\,\mathbb{A}$. The presence of the new quantity $\mathbb{B}_{\kappa_{p(t)}}$ makes the system (2) more complex than the Navier–Stokes system.

The Navier–Stokes equations (1) are nonlinear because of single nonlinear term $\boldsymbol{v} \bullet \nabla \boldsymbol{v}$ in the balance of momentum equation (1b). (Recall that $\frac{\mathrm{d}}{\mathrm{d}t}$ denotes the material time derivative (1f).) Even with such a single nonlinearity, the corresponding dynamical behaviour predicted by the Navier–Stokes model can be very rich and challenging to analyse, just think of *turbulence* phenomenon.

The Oldroyd-B model has, besides the same nonlinear term as the Navier–Stokes model, another nonlinear terms. In particular, the upper convected derivative (3) introduces a *new nonlinearity into the system of governing equations.* This suggests that the dynamical behaviour predicted by the Oldroyd-B model, and for that matters by other models from this class, can be expected to be far more complex than that predicted by the Navier–Stokes model.

2.2.2. *Viscoelastic fluids.* The first question one might ask when dealing with the Oldroyd-B model is why is the corresponding fluid referred to as a visco-*elastic* fluid. The second, closely related question is a physical motivation behind the Oldroyd-B model.

In order to answer these questions, we rewrite the model into two equivalent forms. The introduction of new variables

$$\tilde{p} =_{\text{def}} p + \frac{\mu}{3} \operatorname{Tr} \mathbb{B}_{\kappa_{p(t)}} - \mu, \tag{4a}$$

$$\mathbb{S} =_{\text{def}} \mu \left(\mathbb{B}_{\kappa_{p(t)}} - \mathbb{I} \right), \tag{4b}$$

and the identity $\overset{\triangledown}{\mathbb{I}} = -2\mathbb{D}$, allow us to rewrite the evolution equation for $\mathbb{B}_{\kappa_{p(t)}}$ (2d) and the formulae for the Cauchy stress tensor (1c), (2c) in the form

$$\mathbb{T} = -\tilde{p}\mathbb{I} + 2\nu\mathbb{D} + \mathbb{S}, \tag{5a}$$

$$\nu_1 \overline{\left(\frac{\overset{\triangledown}{\mathbb{S}}}{\mu} \right)} + \mathbb{S} = 2\nu_1 \mathbb{D}. \tag{5b}$$

(Note that for incompressible fluids one is allowed to redefine the pressure at will.) This is the formulation of the Oldroyd-B model frequently used in the mechanics of non-Newtonian fluids, especially if the model is derived by upscaling from a microscopic model based on the concept of dilute polymeric chains dispersed in a Newtonian fluid. The total Cauchy stress $\mathbb{T}$ is understood as a sum of the "solvent" contribution $2\nu\mathbb{D}$ and the extra "polymer" contribution $\mathbb{S}$.

Yet another change of variables

$$\widetilde{\mathbb{S}} =_{\text{def}} \mathbb{S} + 2\nu\mathbb{D} \tag{6}$$

then converts (5) into the form

$$\mathbb{T} = -p\mathbb{I} + \widetilde{\mathbb{S}}, \tag{7a}$$

$$\nu_1 \overline{\left(\frac{\overset{\triangledown}{\widetilde{\mathbb{S}}}}{\mu} \right)} + \widetilde{\mathbb{S}} = 2 \left(\nu_1 + \nu \right) \mathbb{D} + 2\nu_1 \overline{\left(\frac{\overset{\triangledown}{\nu\mathbb{D}}}{\mu} \right)}. \tag{7b}$$

This is the formulation originally obtained by Oldroyd [1950].

If we now consider formulation (7) with $\nu = 0$, which would in the formulation (5) correspond to *zero solvent viscosity*, we see that the formula for $\widetilde{\mathbb{S}}$ reduces to

$$\nu_1 \overline{\left(\frac{\overset{\triangledown}{\widetilde{\mathbb{S}}}}{\mu} \right)} + \widetilde{\mathbb{S}} = 2\nu_1 \mathbb{D}. \tag{8}$$

This resembles the scalar relation

$$\frac{\mathrm{d}F}{\mathrm{d}t} + \frac{F}{T} = E\frac{\mathrm{d}S}{\mathrm{d}t}, \tag{9}$$

where F denotes the "stress" and S denotes the "strain" and E and T are constants. (Recall that $\mathbb{D}$ is the symmetric part of the velocity gradient, hence it can be interpreted, albeit a bit incorrectly, as the "rate of strain" or time derivative of strain.) Formula (9) was used in a remark made by Maxwell [1867] in his study of dynamics of gases, and generalisation of a single scalar equation (9) to the fully nonlinear three-dimensional setting (8) is in fact the main motivation behind Oldroyd [1950] seminal contribution.

Formula (9) justifies the name viscoelastic fluids. Indeed, let us consider a simple mechanical system made of a spring and dashpot (damper) connected in series, see Figure 1. The relation between the applied force F_1 and the strain S_1 for the spring (elastic element) is

$$F_1 = ES_1, \tag{10}$$

where E is a constant, while the relation between the applied force F_2 and the strain S_2 for the daspot (viscous element) reads

$$F_2 = \nu_1 \frac{\mathrm{d}S_2}{\mathrm{d}t}. \tag{11}$$

If the behaviour of the individual elements is specified via (10) and (11), than it is straightforward to find that the relation between the total applied force F and the total strain S is

$$\frac{\mathrm{d}F}{\mathrm{d}t} + \frac{1}{\frac{\nu_1}{E}}F = E\frac{\mathrm{d}S}{\mathrm{d}t}, \tag{12}$$

which is the same as (9). (We have used the fact that $F = F_1 = F_2$ and that $S = S_1 + S_2$.) In this sense, the model (7) is indeed a model for visco-*elastic* fluid—the viscoelastic fluid is a viscous fluid with an additional elastic response. Various simple mechanical analogues made of systems of springs and dashpots in fact serve as a basis for various sophisticated models for viscoelastic response of fluids as well as solids, see, for example, Wineman and Rajagopal [2000].
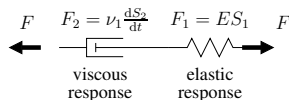
FIGURE 1. Mechanical analog for a viscoelastic rate-type fluid of Maxwell type.

2.2.3. *Stress relaxation and instantaneous elastic response.* Formula (9) also shows that the rate-type viscoelastic models can model the *stress relaxation* effect, and that the fluids described by this model exhibit the *instantaneous elastic response*. Both stress relaxation and instantaneous elastic response are important non-Newtonian effects.

If the strain S is given by the formula

$$S = H(t), \tag{13}$$

where H denotes the Heaviside function,

$$H(t) = \begin{cases} 0, & t < 0, \\ 1, & t \geq 0, \end{cases} \tag{14}$$

then the response force F to such an input is given by the solution to (9) with the right-hand side given by (13). The solution reads

$$F(t) = E\mathrm{e}^{-\frac{t}{T}}H(t). \tag{15}$$

We note that the time derivative of S given by (13) does not exist in the classical sense, and it must be interpreted is a *generalised sense* (typically as a distribution),

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \delta(t - 0). \tag{16}$$

Using (15), we can analyse the force response at $t = 0$. The force instantaneously jumps from zero to $F|_{t=0+} = E$, which is the same response as that of a single elastic spring (10). In this sense we talk about *instantaneous elastic response*[2]. After this event the force exponentially decreases to zero, that is for $t > 0$ we have $F = E\mathrm{e}^{-\frac{t}{T}}$. This process is referred to as the *stress relaxation*.

2.2.4. *Upper convected derivative.* Going from the naive one-dimensional equation (9) to the fully three-dimensional equation (8) requires one to introduce the concept of upper convected derivative. Since the upper convected derivative is the *source of nonlinearity in the model*, it is worthwhile to briefly contemplate on its origin.

If we have an Eulerian tensorial quantity $\mathbb{A}$, and if we want to take its time derivative, we can not simply form the difference quotient

$$\frac{\mathbb{A}(\boldsymbol{x}, t+h) - \mathbb{A}(\boldsymbol{x}, t)}{h}, \tag{17}$$

take the limit $\lim_{h \to 0}$, and declare the limit to be a genuine time derivative. In the difference quotient we need to compare the values of $\mathbb{A}$ that are associated to the same *material point* $\boldsymbol{X}$, and not the same *point in space* $\boldsymbol{x}$. Furthermore, if $\mathbb{A}$ is associated with the given *material point* $\boldsymbol{X}$, not only do we have to track the motion of the material point in space $\boldsymbol{x} = \boldsymbol{\chi}(\boldsymbol{X}, t)$, but we

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[2]This response conforms to the intuition regarding the behaviour of springs and dashpots. If we try to suddenly elongate the spring-dashpot system shown in Figure 1, then the dahspot jams and the elongation takes place only in the spring.

also have to track the corresponding *privileged basis* formed by tangent vectors to material curves and/or normal vectors to material surfaces.

This can be achieved, if we first map all $\mathbb{A}$ back to a reference configuration, then we differentiate as usual in the common reference configuration, and then map the result back to the current configuration. We know that the tangent vectors to material lines are mapped between the reference and the current configuration by the deformation gradient $\mathbb{F}$, and that the normal vectors to the material surfaces are mapped between the reference and the current configuration by $\mathbb{F}^{-\top}$. Consequently, if we want to map a generic tensor $\mathbb{A}$ in an arbitrary current configuration back to the reference configuration, we need to perform the operation

$$\mathbb{F}^{-1}(\boldsymbol{X},t)\mathbb{A}(\boldsymbol{\chi}(\boldsymbol{X},t),t)\mathbb{F}^{-\top}(\boldsymbol{X},t). \tag{18}$$

(The tensor $\mathbb{A}$ in (18) must of a specific type. It must represent a linear mapping that takes a normal to a surface in the current configuration and returns a tangent vector to a material curve in the current configuration. The Cauchy stress tensor and $\mathbb{B}_{\kappa_{p(t)}}$ tensor are of this type.) In this common reference configuration we can differentiate with respect to time as usual, and then we return back to the current configuration, that is we define the derivative as

$$\left.\overset{\triangledown}{\mathbb{A}}(\boldsymbol{x},t)\right|_{\boldsymbol{x}=\boldsymbol{\chi}(\boldsymbol{X},t)} =_{\mathrm{def}} \mathbb{F}(\boldsymbol{X},t)\left[\frac{\mathrm{d}}{\mathrm{d}t}\Big(\mathbb{F}^{-1}(\boldsymbol{X},t)\mathbb{A}(\boldsymbol{\chi}(\boldsymbol{X},t),t)\mathbb{F}^{-\top}(\boldsymbol{X},t)\Big)\right]\mathbb{F}(\boldsymbol{X},t)^{\top}, \tag{19}$$

where we use the standard notation $\boldsymbol{x} = \boldsymbol{\chi}(\boldsymbol{X},t)$ for the *deformation* function, and $\mathbb{F} =_{\mathrm{def}} \frac{\partial \boldsymbol{\chi}(\boldsymbol{X},t)}{\partial \boldsymbol{X}}$ for the deformation gradient. A straightforward algebraic manipulation based on the identity $\frac{\mathrm{d}\mathbb{F}}{\mathrm{d}t} = \mathbb{L}\mathbb{F}$ then reveals that (19) indeed leads to (3).

A reader familiar with differential geometry might recognise the Lie derivative in the above construction, which is indeed the case, see, for example, Stumpf and Hoppe [1997]. Another concepts that lead to the introduction of upper convected derivative are the concept of evolving *natural configuration*, see Rajagopal and Srinivasa [2000] and the concept of objective tensorial rates, see, for example Truesdell and Noll [2004]. (The concept of evolving natural configuration in fact gives a physical meaning of tensor $\mathbb{B}_{\kappa_{p(t)}}$, see Chapter 3 for details.) The reader interested in upper convected derivative and its various generalisations used in continuum mechanics is referred to Bruhns et al. [2004].

2.2.5. *Temperature evolution equation and the second law of thermodynamics.* The original system of equations (2) proposed by Oldroyd [1950], and for that matter many subsequent viscoelastic rate-type models, deals with *mechanical quantities* only. In particular, the temperature evolution equation is missing in the model.

The absence of the corresponding temperature evolution equation indicates that the thermodynamic consistency of the model was not investigated in the early days of viscoelastic rate-type models. The reason is that thermodynamic background is more complicated than that for the Navier–Stokes–Fourier model. Apart from the *kinetic energy* and the *thermal energy*, the energy in a viscoelastic fluid can also take the form of *elastic stored energy*, and one has to deal with mutual conversions between these energy types.

The understanding of thermodynamic of viscoelastic rate-type fluids took a long time, and for simple viscoelastic rate-type models the appropriate temperature evolution equations were not proposed until the last decade of 20th century, see especially Wapperom and Hulsen [1998] and Dressler et al. [1999] and the discussion therein. In fact thermodynamics of more viscoelastic rate-type models is still a subject of research, see, for example, Mackay and Phillips [2019, 2021], both form the theoretical as well as computational perspective.

3. Questions, answers and author's contribution

As indicated in the previous section the analysis of viscoelastic rate-type models provides many opportunities for research work. Particular problems and questions that has been considered in author's own research are for readers convenience listed in Summary 1.

Summary 1: Questions, answers and author's contribution

[**Q1**] What is the status of Oldroyd-B model from the perspective of the concept of *simple fluid*, see Noll [1958]? Can one interpret the Oldroyd-B model and other vicoelastic rate-type models as approximations of a simple fluid with fading memory in the sense of Coleman and Noll [1960]?

The answer is given in [**P7**] and it is based on the concept of *implicit constitutive relations*, see Rajagopal [2003, 2006] and a variant of the approximation theorem by Coleman and Noll [1960].

[**Q2**] The concept of instantaneous elastic response, see Section 2.2.3, requires one to investigate the system response to an input with a jump discontinuity. This is easy to do if the corresponding governing equation is *linear* as in (9). What happens if the governing equation is nonlinear? In the nonlinear case one might face the problem of multiplication of distributions, that is one might need to interpret the terms such as the product of the Heaviside function and the Dirac delta distribution, which is beyond the reach of the classical theory of distributions.

The problem is investigated on an abstract level in [**P8**]. The problem of *multiplication of distributions* is addressed using the *Colombeau algebra*, see Colombeau [1984, 1985, 1992], which is a generalisation of the standard theory of distributions to a nonlinear setting. Applications of the general theory to mechanical systems are given in [**P9**] and [**P10**].

[**Q3**] Governing equations (2) are formulated for mechanical quantities only. What is the corresponding the temperature evolution equation? Is the model consistent with the laws of thermodynamics, in particular with the second law of thermodynamics? What are the corresponding energy storage mechanisms and entropy production mechanisms?

Complete thermodynamic framework for a non-isothermal viscoelastic rate-type model is given in [**P5**]. This work can be seen as a variation to already known results by Wapperom and Hulsen [1998], but from the perspective of the approach developed by Rajagopal and Srinivasa [2000]. Work [**P6**] introduces thermodynamic framework for viscoelastic rate-type fluids with *stress diffusion*, which is a setting wherein a thermodynamic analysis was missing.

[**Q4**] It is nice to have thermodynamically consistent models for viscoelastic fluids, but does it help in the analysis of qualitative behaviour of the corresponding flows? Can thermodynamics help one in *nonlinear* (finite amplitude) *stability analysis* of spatially homogeneous steady states in thermodynamically *isolated systems*, and, more importantly, in *nonlinear stability analysis* of spatially inhomogeneous steady states in thermodynamically *open systems*?

Concerning thermodynamically *isolated systems* the answer is in principle well known—the thermodynamic basis of the models can help one to design candidates for Lyapunov-type functionals for *nonlinear stability analysis* of spatially homogeneous steady states. Yet a rigorous analysis can be still technically challenging. Concerning thermodynamically *open systems* the answer is also positive, basic starting points are discussed in [**P1**]. The method proposed in [**P1**] is then applied in a purely mechanical context in [**P4**], and in a full thermo-mechanical setting in [**P2**] and [**P3**].

Mechanical response

This chapter comments on the answers to questions [**Q1**] and [**Q2**]. We start with [**Q1**] regarding the status of viscoelastic rate-type fluids from the perspective of simple fluids with fading memory.

1. Viscoelastic rate-type fluids from the perspective of simple fluids with fading memory

The main task in mechanics of non-Newtonian fluids is to propose a *constitutive relation* that allows one to determine the value of the Cauchy stress tensor from known values of geometric quantities describing the motion of the fluid, and, if necessary, from other known quantities such as the temperature. In the most primitive case such a geometric quantity might be just the current value of symmetric part of the velocity gradient $\mathbb{D}$.

In influential study Noll [1958] introduced the concept of simple fluid wherein the current value of the Cauchy stress tensor depends on the history of the relative right Cauchy–Green tensor $\mathbb{C}_t(t-s)$. This concept has been later adopted as the key concept in the monumental treatise by Truesdell and Noll [2004]. If we consider and incompressible fluid, the concept of simple fluid formally boils down to the relation

$$\mathbb{T} = -p\mathbb{I} + \mathfrak{F}_{s=0}^{+\infty}(\mathbb{C}_t(t-s)), \tag{20}$$

where p is the indeterminate part of the stress due to the constraint of incompressibility and $\mathfrak{F}_{s=0}^{+\infty}$ is a functional acting on the history of the relative Cauchy–Green tensor. (We follow the terminology introduced by Coleman and Noll [1960], and we do not use the term *functional* for a map from a vector space into its underlying scalar field as it is common in the mathematical literature. What is called *functional* here would be denoted as *operator* in the mathematical literature.) Formula (20) is however not very useful from the practical point of view—it is too general. In practice one needs something more tractable.

In subsequent study Coleman and Noll [1960] make assumptions concerning the memory of the given material, that is they make assumptions on the functional $\mathfrak{F}_{s=0}^{+\infty}$. In particular, they assume:

> Intuitively speaking, the "memory" of the system [...] will "fade away" in time.

Upon formalising this assumption in technical terms, they further assume that the material of interest is subject to *slow processes* only. Using these assumptions it can be then shown that the material response (20) can be—with increasing fidelity—approximated by the constitutive relation wherein the *functional* $\mathfrak{F}_{s=0}^{+\infty}$ is replaced by an algebraic combination of Rivlin–Ericksen tensors[1] $\mathbb{A}_n$. This then leads to observation that a whole cascade of the so-called *differential-type* models can be seen as approximations to the "exact" model (20) in slow processes, see Coleman and Noll [1960]

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[1]We recall that the Rivlin–Ericksen tensors $\mathbb{A}_n$ are defined in terms of the derivatives of the relative Cauchy–Green tensor

$$\mathbb{A}_n(\boldsymbol{x},t) =_{\text{def}} \left.\frac{\mathrm{d}^n\mathbb{C}_t(\boldsymbol{x},\tau)}{\mathrm{d}\tau^n}\right|_{\tau=t}, \tag{21}$$

and that they can be computed by the recursive formula

$$\mathbb{A}_1 = 2\mathbb{D}, \tag{22a}$$

$$\mathbb{A}_n = \frac{\mathrm{d}\mathbb{A}_{n-1}}{\mathrm{d}t} + \mathbb{A}_{n-1}\mathbb{L} + \mathbb{L}^\top\mathbb{A}_{n-1}, \tag{22b}$$

.

and Truesdell and Noll [2004] for details. For example, the so-called *second order incompressible fluid* is given by the formula

$$\mathbb{T} = -p\mathbb{I} + \nu\mathbb{A}_1 + \beta\mathbb{A}_1^2 + \gamma\mathbb{A}_2, \tag{23}$$

where ν, β and γ are constants.

Neither of these approximating models however resembles the rate-type Oldroyd-B model (7b) where one works not only with the time derivatives of the geometric quantities but also with the time derivatives of the (part of) stress tensor. This brings us back to question [**Q1**]. In fact question on relations between various concepts in mechanics of non-Newtonian fluids has always troubled the community, see, for example, Walters [1970].

In [**P7**] we reconcile the concept of fading memory and the concept of viscoelastic rate-type fluid. We appeal to the concept of *implict constitutive relations*, see Rajagopal [2003, 2006]. The concept, with a bit of oversimplification, claims that the relation between the stress tensor and the geometrical quantities should take the generalised form

$$\mathfrak{H}_{s=0}^{+\infty} \left(\mathbb{T}(t-s), \mathbb{C}_t\left(t-s\right) \right) = \mathbb{0}. \tag{24}$$

A proper nontrivial modification of the approximation procedure introduced by Coleman and Noll [1960] then reveals, see [**P7**] for details, that the viscoelastic rate-type models can be seen as approximations of the "exact" and "all-encompassing" model (24). For example, if we consider only slow processes, then the model

$$\mathbb{T} = -p\mathbb{I} + \mathbb{S}, \tag{25a}$$

$$b_0 \left(\operatorname{Tr} \mathbb{S}\right) \mathbb{I} + b_1 \mathbb{S} + 2b_3 \mathbb{D} + b_4 \left(\operatorname{Tr} \overset{\triangledown}{\mathbb{S}}\right) \mathbb{I} + b_5 \overset{\triangledown}{\mathbb{S}} = \mathbb{0}, \tag{25b}$$

where $\{b_i\}_{i=0}^5$ are constants, is a first order approximation of (24), and the standard Maxwell model (8) is clearly a special case of (25). The main technical issue in the analysis [**P7**] is the introduction of the upper convected derivative of stress; this is achieved by the application of a variant of Coleman and Noll [1960] approximation procedure in a convected coordinate system and subsequent transformation back to the fixed-in-space coordinate system.

2. Multiplication of distributions and response to step input

Question [**Q2**] deals with the response of systems governed by ordinary differential equations to *step inputs*. As indicated in Section 2.2.3 in Chapter 1 such a problem arises in analysis of *creep* and *stress relaxation* experiments with viscoelastic materials, see, for example, Wineman and Rajagopal [2000].

In principle we are facing the problem outlined in Figure 1. We have a system governed by a nonlinear ordinary differential equation of the type

$$f\left(\varepsilon, \sigma, \frac{\mathrm{d}\varepsilon}{\mathrm{d}t}, \frac{\mathrm{d}\sigma}{\mathrm{d}t}, \frac{\mathrm{d}^2\varepsilon}{\mathrm{d}t^2}, \frac{\mathrm{d}^2\sigma}{\mathrm{d}t^2}\right) = 0, \tag{26}$$

where f is a given scalar function and ε and σ are functions of time. (Here the notation ε and σ suggests the physical interpretation—the symbol ε denotes the strain and the symbol σ denotes the stress.) We control one of the quantities ε or σ—for specificity let us assume that we control ε—and we refer to this quantity as the *input*. The *response* quantity is then σ, which is given as a solution to (26) for the given input ε. Typically, the input ε is a piecewise smooth function with a *jump discontinuity* at time t_{j}, while the response σ is expected, in a reasonable physical system, to have a jump at time t_{j} as well. An intricate question then arises—knowing the height of the jump in the input, what is the height of the jump in the response?

In fact, once the jump event is over, we are typically dealing with a standard ordinary differential equation, which is a well studied problem. The only thing we need to know are the initial conditions for this differential equation. This means that we need to know, depending on the order of the governing equation, the initial value of the response function at time t_{j} (the height of the jump) and the slope of the response curve at time t_{j} of and so forth. Clearly, this is the only *conceptually difficult part of the problem*, since once we pass the jump event we are within the realm of standard theory of ordinary differential equations.
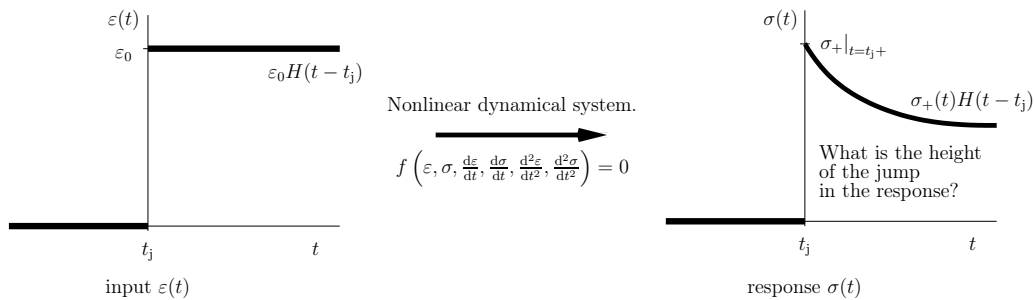
FIGURE 1. Response of a system governed by a nonlinear ordinary differential equation to a step input.

If the material response is *linear*—the function f specifying the governing equation (26) is linear—then the analysis of response to jump input is straightforward. Equation (26)—which is in this case a linear equation—is interpreted and solved in the sense of *distributions*, see Schwartz [1966]. In particular the time derivatives of functions with jump discontinuities simply generate Dirac delta distributions.

If the material response is *nonlinear*—the function f specifying the governing equation (26) is nonlinear—the story changes completely. It is impossible to use the standard theory of distributions since the nonlinear operations with standard distributions are not defined. Consequently, it is not clear how to interpret the equation at all. Worse than that, the lack of nonlinear operations in the standard theory of distributions is not a matter of exaggerated rigour. The multiplication of standard distributions is not defined for a good reason, see Schwartz [1954], since it could lead to various paradoxes.

We have first encountered this problem in Průša and Rajagopal [2011], where we have studied the response of a material described by the constitutive relation

$$\sigma + \lambda_1(\sigma)\frac{\mathrm{d}\sigma}{\mathrm{d}t} + \lambda_2(\sigma)\frac{\mathrm{d}^2\sigma}{\mathrm{d}t^2} = 2\mu_1(\sigma)\frac{\mathrm{d}\varepsilon}{\mathrm{d}t} + 2\mu_2(\sigma)\frac{\mathrm{d}^2\varepsilon}{\mathrm{d}t^2}, \tag{27}$$

where $\lambda_1, \lambda_2, \mu_1$ and μ_2 are given functions. (This material can be seen as a generalisation of Burgers fluid model.) In Průša and Rajagopal [2011] we in principle apply a straightforward naive approach to the problem. The input—this time the function σ—with a jump discontinuity is with a an increasing fidelity *approximated via a sequence of smooth inputs* $\{\sigma_n\}_{n=1}^{\infty}$ without jump discontinuity, and we study the corresponding sequence of responses $\{\varepsilon_n\}_{n=1}^{\infty}$. Under certain conditions on functions $\lambda_1, \lambda_2, \mu_1$ and μ_2, we then show that the sequence of responses $\{\varepsilon_n\}_{n=1}^{\infty}$ has a limit, and this limit is interpreted as a response to the input with jump discontinuity. Subsequently, we interpret this limit process in the framework of *Colombeau algebra of generalised functions*.

Colombeau algebra, see Colombeau [1984, 1985, 1992], Rosinger [1990, 1987] and Biagioni [1990], is a generalisation of the standard theory of distributions into the nonlinear setting. Unlike in the standard theory of distributions, the generalised functions are not constructed as linear functionals whose action on smooth "test" functions is known. The approach to generalised functions is completely different in Colombeau algebra.

On a very informal level, the approach to the generalised functions in Colombeau algebra is based on the interpretation of generalised functions as *collections of smooth functions that provide appropriate approximation of the target non-smooth object* (function with jump discontinuity, standard distribution). All the operations such as the multiplication and the differentiation are then done at the level of smooth approximations, and the resulting new collection of smooth functions is then declared to represent the result of the multiplication or differentiation between the target objects (function with jump discontinuity, standard distribution). Furthermore, Colombeau algebra introduces two types of equality, a strict one, and the so-called *equality in the sense of association*.

The equality in the sense of association basically means that two generalised functions are equal up to some "microscopic" features such as the structure of the jump discontinuity. (Asymptotic behaviour of the smoothed approximations at the jump discontinuity.) In particular, the equality in the sense of association allows one to formalise statements such as $H^2 = H$, where H is the Heaviside

function. Careful balance between the definitions of multiplication and differentiation and the strict equality and the equality in the sense of association then leads to the so-called *coupled calculus*, which allows one, amongst other, to define and study a generalised solution to the equations of type (26), see [**P8**] for a concise summary.

From the user perspective, the rules of the *coupled calculus* in Colombeau algebra encapsulate all the details concerning the sequential approximations, and one can work on a symbolic level with "sharp" objects only. For example, one can directly work with symbolic expressions of the type $\frac{\mathrm{d}H}{\mathrm{d}t} = \delta$, and there is no need to go into the details regarding the sequential interpretation thereof.

In [**P8**] we have adopted this approach, and we have studied generalised solutions to equations

$$a(\varepsilon, \sigma)\sigma + \frac{\mathrm{d}\sigma}{\mathrm{d}t} = b(\varepsilon, \sigma)\varepsilon + c(\varepsilon, \sigma)\frac{\mathrm{d}\varepsilon}{\mathrm{d}t}, \tag{28}$$

and

$$\sigma + a(\sigma, \varepsilon)\frac{\mathrm{d}\sigma}{\mathrm{d}t} + \tilde{b}\frac{\mathrm{d}^2\sigma}{\mathrm{d}t^2} = 2c(\sigma, \varepsilon)\frac{\mathrm{d}\varepsilon}{\mathrm{d}t} + 2\tilde{d}\frac{\mathrm{d}^2\varepsilon}{\mathrm{d}t^2}, \tag{29}$$

where a, b and c are given functions and b and d are constants. In particular we have been interested in the response to a step input, and we have derived theorems that explicitly allow one to find the height of the jump in (28), and the height of the jump and the initial slope after the jump event in (29), see [**P8**].

For example, concerning (28) the corresponding theorem reads as follows.

THEOREM 10 (Solution of equation $a(\varepsilon, \sigma)\sigma + \frac{\mathrm{d}\sigma}{\mathrm{d}t} = b(\varepsilon, \sigma)\varepsilon + c(\varepsilon, \sigma)\frac{\mathrm{d}\varepsilon}{\mathrm{d}t}$). *Let us consider a system governed by ordinary differential equation*

$$a(\varepsilon, \sigma)\sigma + \frac{\mathrm{d}\sigma}{\mathrm{d}t} = b(\varepsilon, \sigma)\varepsilon + c(\varepsilon, \sigma)\frac{\mathrm{d}\varepsilon}{\mathrm{d}t}, \tag{30}$$

where functions $a(\varepsilon, \sigma)$, $b(\varepsilon, \sigma)$ and $c(\varepsilon, \sigma)$ are smooth functions such that ordinary differential equation (30) has for the given smooth ε a unique smooth solution σ. If (30) is understood in the generalised sense of Colombeau algebra as

$$a(\boldsymbol{\varepsilon}, \boldsymbol{\sigma})\boldsymbol{\sigma} + \frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}t} \approx b(\boldsymbol{\varepsilon}, \boldsymbol{\sigma})\boldsymbol{\varepsilon} + c(\boldsymbol{\varepsilon}, \boldsymbol{\sigma})\frac{\mathrm{d}\boldsymbol{\varepsilon}}{\mathrm{d}t}, \tag{31}$$

then the response σ of the system governed by (30) to the step input ε

$$\varepsilon = \begin{cases} 0, & t < 0, \\ \tilde{\varepsilon}(t), & t \geq 0, \end{cases} \tag{32}$$

where $\tilde{\varepsilon}$ is a smooth function, is given by the function

$$\sigma = \begin{cases} 0, & t < 0, \\ \tilde{\sigma}(t), & t \geq 0. \end{cases} \tag{33}$$

(The function σ is interpreted as an element in Colombeau algebra via the canonical embedding.) Function $\tilde{\sigma}$ is for $t > 0$ a solution to the ordinary differential equation

$$a(\tilde{\varepsilon}, \tilde{\sigma})\tilde{\sigma} + \frac{\mathrm{d}\tilde{\sigma}}{\mathrm{d}t} = b(\tilde{\varepsilon}, \tilde{\sigma})\tilde{\varepsilon} + c(\tilde{\varepsilon}, \tilde{\sigma})\frac{\mathrm{d}\tilde{\varepsilon}}{\mathrm{d}t} \tag{34a}$$

$$\tilde{\sigma}|_{t=0_+} = \sigma_0. \tag{34b}$$

The initial condition σ_0 in (34)—that is the height of the jump in the response—is obtained by evaluating the solution ς of the ordinary differential equation

$$\frac{\mathrm{d}\varsigma}{\mathrm{d}\epsilon} = c(\epsilon, \varsigma), \tag{35a}$$

$$\varsigma|_{\epsilon=0} = 0, \tag{35b}$$

at point $\epsilon = \varepsilon_0$, that is $\sigma_0 = \varsigma|_{\epsilon=\varepsilon_0}$, where $\varepsilon_0 =_{\mathrm{def}} \tilde{\varepsilon}|_{t=0_+}$ denotes the height of the jump in the input.

We see that the height of the jump in the response function (34b), that is the initial condition for the standard ordinary differential equation after the jump event, is indeed explicitly identified. The height of the jump is given by the solution to an auxilliary differential equation (35).

Note that the Colombeau algebra setting does not always lead to a solution to the corresponding differential equation. For some systems, see Průša and Rajagopal [2011] for details, the response to the sequence of approximated inputs *does not converge*. This means that the solution based on the equality in the sense of association does not exist. However, such a behaviour has a nice physical interpretation. In such a case the response is sensitive to "microscopic" details at the jump discontinuity, meaning that the particular features of the *smoothing* procedure *does* matter. (In real setting the jump discontinuity in strain is an idealisation of some fast continuous transition. Hence we are not in principle working with a jump discontinuity but with its particular "smoothed" version.) The details of the smoothing procedure are not smeared out, instead they are magnified, and if we want to know the response of the system, we must provide the detailed description of the jump discontinuity.

The abstract results obtained in [**P8**] are then used in subsequent works [**P9**] and [**P10**]. In [**P9**] we show how to apply the theory in investigation of the response of spring–dashpot–mass systems wherein the individual mechanical elements are described by nonlinear constitutive relations, see Figure 2 for a sketch of such a system. Finally, in [**P10**] we investigate the response of a viscoelastic fluid in a fully three-dimensional setting, in particular we show how to apply the theory in the case of suddenly started squeeze flow, see Figure 3 for a sketch of such a system.
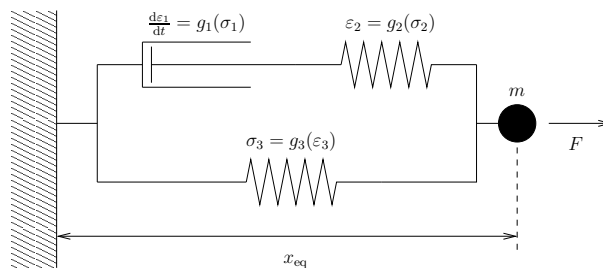
FIGURE 2. Nonlinear spring–dashpot system with an attached mass.

(A) Constant mass of the sample between the plates.

(B) Constant contact area between the sample and the plates.
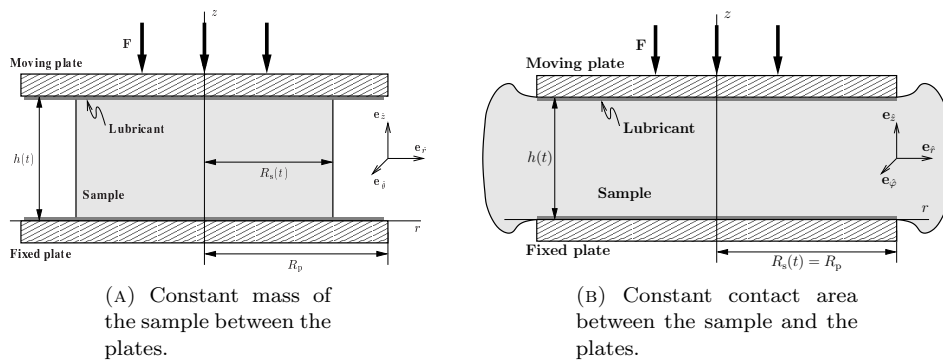
FIGURE 3. Lubricated squeeze flow. Axisymmetric sample is compressed by two parallel plates with lubricated surfaces ensuring the perfect slip boundary condition on the sample-plate interfaces.

Thermodynamics

This chapter provides explanatory comments to the technical results regarding question [**Q3**], that is the question regarding thermodynamic background of some viscoelastic rate-type models.

The objective is to provide thermodynamic background to the classical viscoelastic rate type models such as the Oldroyd-B model

$$\operatorname{div} \boldsymbol{v} = 0, \tag{36a}$$

$$\rho \frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = \operatorname{div} \mathbb{T} + \rho \boldsymbol{b}, \tag{36b}$$

$$\frac{\nu_1}{\mu} \overset{\triangledown}{\mathbb{S}} + \mathbb{S} = 2\nu_1 \mathbb{D}, \tag{36c}$$

$$\mathbb{T} = -p\mathbb{I} + 2\nu \mathbb{D} + \mathbb{S}, \tag{36d}$$

where ν, μ and ν_1 are constants. (See Section 2.2 in Chapter 1 for a discussion of Oldroyd-B model. Compared to (5) we use the symbol p instead of $\tilde{p}$. This change is inconsequential.) As we have already noted certain thermodynamic background for Oldroyd-B model existed prior to our work, and our contribution [**P5**] can be thus seen as a reformulation and generalisation of known results from a different perspective, that is using the concept of *evolving natural configuration.* Furthermore, in [**P5**] we also investigate the impact of *temperature dependent* material parameter μ on the response of the given fluid. This is an important feature, since the *elastic* response of the fluid then exhibits thermo-mechanical effects such as the Gough–Joule effect in elastic solids, see Gough [1805], Joule [1859] and, for example, a newer contribution by Anand [1996].

But our contribution goes beyond thermodynamic analysis of Oldroyd-B model and other qualitatively similar models, no matter whether with or without temperature dependent material parameters. In [**P6**] and Dostalík et al. [2019a] we provide thermodynamic background for viscoelastic rate-type models with *stress diffusion*, that is for variants of the model

$$\operatorname{div} \boldsymbol{v} = 0, \tag{37a}$$

$$\rho \frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = \operatorname{div} \mathbb{T} + \rho \boldsymbol{b}, \tag{37b}$$

$$\frac{\nu_1}{\mu} \overset{\triangledown}{\mathbb{S}} + \mathbb{S} = 2\nu_1 \mathbb{D} + \varepsilon \Delta \mathbb{S}, \tag{37c}$$

$$\mathbb{T} = -p\mathbb{I} + 2\nu \mathbb{D} + \mathbb{S}. \tag{37d}$$

For such models thermodynamic background was unknown prior to our work.

The term $\Delta \mathbb{S}$ is referred to as the *stress diffusion* term, and there are several reasons for this qualitative modification of the standard Oldroyd-B model. First, the presence of the term guarantees some qualitative properties of corresponding flows, in particular in modelling of *shear banding phenomenon.* Second, if the model is carefully derived using the micro-macro models based on the concept of dilute polymeric fluids, then the stress diffusion term naturally appears. Third, it can be expected that (37) has better mathematical properties than (36). For further discussion concerning the stress diffusion term see [**P6**], up-to-date comments can be found in Varchanis et al. [2022], while seminal paper on stress diffusion term is El-Kareh and Leal [1989].

1. Concept of evolving natural configuration

We want thermodynamic background for viscoelastic rate-type models to be *purely phenomenological*, which means that we want to work with macroscopic quantities/concepts only.

In particular, we do not want to refer to the concept of *conformation tensor*. This concept is used in theory of dilute polymeric fluids, and the conformation tensor is a quantity describing the configuration of polymeric chains and can be related to quantity $\mathbb{B}_{\kappa_{p(t)}}$, for details see, for example, Bird et al. [1987a], Grmela and Carreau [1987], Beris and Edwards [1994] and Phan-Thien [2013]. (The concept of conformation tensor essentially goes back to Kramers [1946].) While the use of *conformation tensor* is perfectly fine and insightful in the case of dilute polymeric fluids, polymeric fluids represent only one class of fluids that on macroscopic level exhibit viscoelastic behaviour. Indeed, fluid substances such as blood, Thurston [1972], asphalt binders, Narayan et al. [2016], or Earth's mantle, Harder [1991] and Moresi et al. [2002], exhibit viscoelastic behaviour as well, but their internal structure is far out from sparsely scattered polymeric chains flowing in a solvent, hence the concept of *conformation tensor* is of no use here.
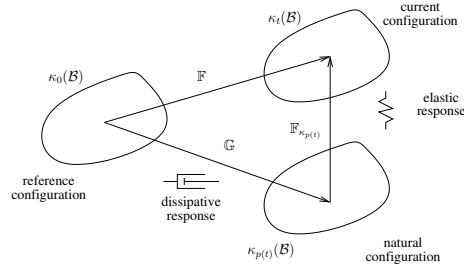

FIGURE 1. Viscoelastic fluid – kinematics of evolving natural configuration.

The right concept for purely phenomenological analysis seems to be the concept of *evolving natural configuration*. The concept of *evolving natural configuration* allows one to generalise simple phenomenological spring–dashpot models, see Figure 1 in Chapter 1, to the setting of continuous media. The key idea, see Rajagopal and Srinivasa [2000], is that the response of the given fluid is decomposed to a dissipative part (dashpot) and an elastic part (spring), see Figure 1. (On the formal level, this is similar idea as that in the celebrated paper Lee [1969] on finite elasto-plastic deformation of solids.) The intermediate configuration $\kappa_{p(t)}(\mathcal{B})$ is referred to as the *natural configuration*, and it corresponds to the configuration the material will take after instantaneous unloading. (Recall that such a process is—according to the insight from spring-dashpot model—an elastic process. See Section 2.2.3 in Chapter 1.) The tensor $\mathbb{B}_{\kappa_{p(t)}}$ that appears in governing equations (36) is then the left Cauchy–Green tensor associated to the elastic part of the response,

$$\mathbb{B}_{\kappa_{p(t)}} =_{\mathrm{def}} \mathbb{F}_{\kappa_{p(t)}} \mathbb{F}^{\top}_{\kappa_{p(t)}}. \tag{38}$$

This subtle shift in interpretation of the extra tensorial quantity $\mathbb{B}_{\kappa_{p(t)}}$ has been largely appreciated by the research community in non-Newtonian fluids, and the paper Rajagopal and Srinivasa [2000] has been included in the 40th Anniversary Article Collection of Journal of Non-Newtonian Fluid Mechanics. We follow this interpretation of $\mathbb{B}_{\kappa_{p(t)}}$ in our works.

2. Thermomechanical response of standard viscoelastic rate-type fluids

The thermodynamic analysis is based on the assumption that the given material is fully characterised by its *energy storage ability* and *entropy production ability*, see Rajagopal and Srinivasa [2004] for a thorough discussion thereof. The energy storage ability is characterised by the choice of the Helmholtz free energy function, while the entropy production ability is characterised by the choice of entropy production function. (The Helmholtz free energy can by substituted by an equivalent thermodynamic potential.) Both these functions are *scalar* functions, and their choice indeed implies the constitutive relations for the *tensorial* quantities such as the Cauchy stress tensor and *vectorial* quantities such as the heat flux.

In order to develop phenomenological models for viscoelastic rate-type fluids, we thus need to properly specify the *energy storage ability* and *entropy production ability* of the given fluid. Concerning the Helmholtz free energy[1], we split it to purely thermal part ψ^{thermal} and to deformation dependent part ψ^{mech}.

For the thermal part ψ^{thermal} we can use the classical formula

$$\psi^{\text{thermal}} =_{\text{def}} -c_{\text{V,ref}}\theta\left(\ln\frac{\theta}{\theta_{\text{ref}}} - 1\right), \tag{39}$$

where θ denotes the temperature and θ_{ref} is a reference temperature value (a constant) and $c_{\text{V,ref}}$ is a constant. Formula (39) leads to a material with the *specific heat capacity at constant volume* equal to the constant $c_{\text{V,ref}}$.

Concerning the energy storage mechanisms related to the deformation, that is concerning the specification of ψ^{mech}, it is also almost obvious what to do. We assume that the energy storage mechanisms are related to the *elastic response* of the fluid, and we characterise the energy storage ability by the same manner as in standard theory of Green elastic (hyperelastic solids) solids. Instead of the full left Cauchy–Green tensor for the *full response* $\mathbb{B} =_{\text{def}} \mathbb{F}\mathbb{F}^{\top}$, which is the right choice for solid materials, we however use the left Cauchy–Green tensor $\mathbb{B}_{\kappa_{p(t)}}$ associated to the *elastic part* of fluid response. (For a list of popular stored energy functions for hyperelastic materials see, for example, Marckmann and Verron [2006], Destrade et al. [2017] or Mihai and Goriely [2017].) Note that ψ^{mech} can still depend on the temperature. It can be, for example, proportional to the temperature such as in the classical entropic elasticity, see, for example, Ericksen [1998] and Anand [1996].

Regarding the basic incompressible Oldroyd-B model (36) with temperature independent material parameters, the following choice of Helmholtz free energy is an appropriate one,

$$\psi(\theta, \mathbb{B}_{\kappa_{p(t)}}) =_{\text{def}} \psi^{\text{thermal}}(\theta) + \psi^{\text{mech}}(\theta, \mathbb{B}_{\kappa_{p(t)}}), \tag{40a}$$

$$\psi^{\text{thermal}}(\theta) =_{\text{def}} -c_{\text{V,ref}}\theta\left(\ln\frac{\theta}{\theta_{\text{ref}}} - 1\right), \tag{40b}$$

$$\psi^{\text{mech}}(\theta, \mathbb{B}_{\kappa_{p(t)}}) =_{\text{def}} \frac{\mu}{2\rho}\left(\text{Tr}\,\mathbb{B}_{\kappa_{p(t)}} - 3 - \ln\det\mathbb{B}_{\kappa_{p(t)}}\right), \tag{40c}$$

see Málek et al. [2015].

Having identified the Helmholtz free energy, we can proceed with the entropy production. If the Helmholtz free energy $\psi = \psi(\theta, y_1, \ldots, y_N)$ is given as a function of temperature θ and other state variables denoted as $\{y_i\}_{i=1}^{N}$, then the entropy evolution equation in the Eulerian description reads

$$\rho\frac{\mathrm{d}\eta}{\mathrm{d}t} + \text{div}\left(\frac{\boldsymbol{j}_q}{\theta}\right) = \frac{1}{\theta}\left\{\mathbb{T}:\mathbb{D} - \rho\sum_{i=1}^{N}\frac{\partial\psi}{\partial y_i}\frac{\mathrm{d}y_i}{\mathrm{d}t}\right\} - \boldsymbol{j}_q\bullet\frac{\nabla\theta}{\theta^2}, \tag{41}$$

where the symbol η denotes the entropy and $\boldsymbol{j}_q$ denotes the heat flux. (For the derivation of (41) see Truesdell and Noll [1965], Müller [1985] or any standard book on continuum thermodynamics. Here we follow the notation used in Málek and Průša [2018].) The terms on the right-hand side of (41) are referred to as the *entropy production terms*, and the objective is to propose constitutive relations in such a way that the right-hand side of (41) is positive. In particular we are interested in the specification of a formula for the Cauchy stress tensor.

In our case, the entropy evolution equation reduces to

$$\rho\frac{\mathrm{d}\eta}{\mathrm{d}t} + \text{div}\left(\frac{\boldsymbol{j}_q}{\theta}\right) = \frac{1}{\theta}\left\{\mathbb{T}:\mathbb{D} - \rho\frac{\partial\psi}{\partial\mathbb{B}_{\kappa_{p(t)}}}:\frac{\mathrm{d}\mathbb{B}_{\kappa_{p(t)}}}{\mathrm{d}t}\right\} - \boldsymbol{j}_q\bullet\frac{\nabla\theta}{\theta^2} \tag{42}$$

Following Rajagopal and Srinivasa [2000] the next step is—in a nutshell—based on the prescription of entropy production. A generic entropy evolution equation must read

$$\rho\frac{\mathrm{d}\eta}{\mathrm{d}t} + \text{div}\,\boldsymbol{j}_\eta = \xi, \tag{43}$$

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[1]The Helmholtz free energy ψ is introduced as *energy density per unit mass*. This means that the physical dimension of ψ is $[\psi] = \text{J/kg}$, and that the net Helmholtz free energy is obtained by the integration over the current configuration of the body of interest, that is $\int_{\Omega}\rho\psi\,\mathrm{d}v$. (Similarly for the entropy.)

where $\boldsymbol{j}_\eta$ denotes the *entropy flux* and ξ denotes the *entropy production*, $\xi \geq 0$. In order to characterise the entropy production abilities of the material, we *prescribe* the entropy production ξ in (43), and then we "compare" it with the right-hand side (41), that is with the entropy production that is implied by the previous choice of the Helmholtz free energy. For example, if we choose

$$\xi =_{\mathrm{def}} \frac{1}{\theta} \left\{ 2\nu \mathbb{D}_\delta : \mathbb{D}_\delta + \frac{\mu^2}{2\nu_1} \mathrm{Tr}\left[\mathbb{B}_{\kappa_{p(t)}} + \mathbb{B}_{\kappa_{p(t)}}^{-1} - 2\mathbb{I} \right] \right\} + \kappa \frac{\nabla\theta \bullet \nabla\theta}{\theta^2}, \tag{44}$$

then we can, after some manipulation, see Málek and Průša [2018] or [**P5**] for details, identify the formulae for the heat flux $\boldsymbol{j}_q$ and the Cauchy stress tensor as

$$\mathbb{T} =_{\mathrm{def}} -p\mathbb{I} + 2\nu\mathbb{D}_\delta + \mu\left(\mathbb{B}_{\kappa_{p(t)}} \right)_\delta, \tag{45a}$$

$$\boldsymbol{j}_q =_{\mathrm{def}} -\kappa\nabla\theta, \tag{45b}$$

while the formula for the time derivative of $\mathbb{B}_{\kappa_{p(t)}}$ must read

$$\nu_1 \overline{\mathbb{B}_{\kappa_{p(t)}}}^{\triangledown} = -\mu\left[\mathbb{B}_{\kappa_{p(t)}} - \mathbb{I} \right]. \tag{45c}$$

The temperature evolution equation is then obtained from (42) and the fact that $\eta = -\frac{\partial\psi}{\partial\theta}(\theta, \mathbb{B}_{\kappa_{p(t)}})$. We note that if the shear modulus μ is temperature dependent, then formulae (45) remain the same. (The thermodynamic background for the Oldroyd-B model is summarised in Summary 2.) However, the corresponding temperature evolution equation is different than that in the constant shear modulus case. The impact of temperature dependent shear modulus μ on fluid dynamic is discussed in [**P5**]. A list of Helmholtz free energies and entropy production for various popular models is given in Dostalík et al. [2019a]—an updated version posted at arXiv.org (arXiv:1902.07983) corrects some misprints in the published paper.

Finally, we emphasise that the specification of energy storage mechanism in terms of the Helmholtz free energy is not the only option. Other thermodynamic potentials, in particular the Gibbs free energy, might be used as well. This is of interest from the perspective of new developments in theory of elastic solids, see Muliana et al. [2018], Bustamante and Rajagopal [2020], Průša et al. [2020] and references therein, where the use of Gibbs potential seem to lead, in some case, to better phenomenological models than in the standard setting based on the Helmholtz free energy. The point is that although the descriptions based on different thermodynamic potentials might be formally equivalent, the particular *formulae* might be simpler in one of the descriptions.

The use of Gibbs potential in theory of viscoelastic rate-type models, which is a novel contribution to the field, is investigated in Průša and Rajagopal [2021]. The thermodynamic background of Oldroyd-B mode is, from the perspective of Gibbs free energy, is summarised in Summary 3. Interestingly, the main kinematic quantity in the Gibbs description is the Hencky strain tensor $\mathbb{H}_{\kappa_{p(t)}}$ associated to the elastic response of the fluid $\mathbb{H}_{\kappa_{p(t)}} =_{\mathrm{def}} \frac{1}{2}\ln\mathbb{B}_{\kappa_{p(t)}}$, which opens up the possibility to seamlessly formulate models that are from the very beginning working with the log-conformation tensor, see Fattal and Kupferman [2004]. This is a task for future investigation.

3. Thermomechanical response of viscoelastic rate-type fluids with stress diffusion

Viscoelastic rate-type models (37) with the stress diffusion term $\Delta\mathbb{S}$ are challenging from the modelling perspective. Following the assumption that each material is characterised by its energy storage mechanisms and entropy production mechanisms, we must make a decision regarding the origin of the stress diffusion term. Either we can consider the stress diffusion term to be a consequence of a *new energy storage mechanism* or of a *new entropy production mechanism*.

In [**P6**] we investigate both options. If we want to interpret the stress diffusion term as a consequence of a new energy storage mechanism, we need to specify the corresponding Helmholtz free energy. Assuming that the standard Helmholtz free energy (40) contains an *additional nonlocal term*, that is if we set

$$\psi =_{\mathrm{def}} \widetilde{\psi}(\theta, \rho) + \frac{\mu}{2\rho}\left(\mathrm{Tr}\,\mathbb{B}_{\kappa_{p(t)}} - 3 - \ln\det\mathbb{B}_{\kappa_{p(t)}} \right) + \frac{\tilde{\mu}(\theta)}{2\rho}\left| \nabla\,\mathrm{Tr}\,\mathbb{B}_{\kappa_{p(t)}} \right|^2 \tag{46}$$

then we indeed get a diffusion term in the evolution equation for $\mathbb{B}_{\kappa_{p(t)}}$, and consequently in the evolution equation for $\mathbb{S}$, see Section 2.2 in Chapter 1 for various forms of governing equations for

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Summary 2: Incompressible Oldroyd-B model via Helmholtz free energy

Specific Helmholtz free energy:

$$\psi(\theta, \mathbb{B}_{\kappa_{p(t)}}) =_{\text{def}} \psi_{\text{thermal}}(\theta) + \frac{\mu(\theta)}{2\rho}\left(\operatorname{Tr}\mathbb{B}_{\kappa_{p(t)}} - 3 - \ln\det\mathbb{B}_{\kappa_{p(t)}}\right)$$

$$\psi_{\text{thermal}}(\theta) =_{\text{def}} -c_{\text{V,ref}}\theta\left(\ln\frac{\theta}{\theta_{\text{ref}}} - 1\right).$$

Entropy production:

$$\xi = \frac{1}{\theta}\left\{2\nu\mathbb{D}_\delta : \mathbb{D}_\delta + \frac{\mu(\theta)^2}{2\nu_1}\operatorname{Tr}\left[\mathbb{B}_{\kappa_{p(t)}} + \mathbb{B}_{\kappa_{p(t)}}^{-1} - 2\mathbb{I}\right]\right\} + \kappa\frac{\nabla\theta \bullet \nabla\theta}{\theta^2}$$

Material parameters: $c_{\text{V,ref}}$ specific heat at constant volume – positive constant; $\mu(\theta)$ shear modulus – nonnegative function, typically proportional to θ; ν, ν_1 viscosity – nonnegative functions of the primitive variables, typically constants; κ thermal conductivity – nonnegative function of the primitive variables, typically constant

Evolution equations (mechanical variables p, $\boldsymbol{v}$, $\mathbb{B}_{\kappa_{p(t)}}$ and thermal variable θ):

$$\operatorname{div}\boldsymbol{v} = 0$$

$$\rho\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = \operatorname{div}\mathbb{T} + \rho\boldsymbol{b}$$

$$\nu_1\overset{\triangledown}{\overline{\mathbb{B}_{\kappa_{p(t)}}}} = -\mu(\theta)\left[\mathbb{B}_{\kappa_{p(t)}} - \mathbb{I}\right]$$

$$-\rho\theta\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\psi}{\partial\theta}(\theta, \mathbb{B}_{\kappa_{p(t)}})\right) = \operatorname{div}(\kappa\theta) + 2\nu\mathbb{D}_\delta : \mathbb{D}_\delta + \frac{\mu(\theta)^2}{2\nu_1}\operatorname{Tr}\left[\mathbb{B}_{\kappa_{p(t)}} + \mathbb{B}_{\kappa_{p(t)}}^{-1} - 2\mathbb{I}\right]$$

Cauchy stress tensor:

$$\mathbb{T} = -p\mathbb{I} + 2\nu\mathbb{D}_\delta + \mu(\theta)\left(\mathbb{B}_{\kappa_{p(t)}}\right)_\delta$$

Thermodynamical relations:

$$\eta = -\frac{\partial\psi}{\partial\theta}(\theta, \mathbb{B}_{\kappa_{p(t)}})$$

Left Cauchy–Green tensor $\mathbb{B}_{\kappa_{p(t)}}$ and Hencky strain tensor $\mathbb{H}_{\kappa_{p(t)}}$ associated to the elastic response:

$$\mathbb{B}_{\kappa_{p(t)}} = \mathrm{e}^{2\mathbb{H}_{\kappa_{p(t)}}}$$

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viscoelastic rate-type fluids. (Note that (46) is written for a compressible fluid.) The terminology "nonlocal term" is here used for a gradient term; this is a common practice. The corresponding evolution equation for $\mathbb{B}_{\kappa_{p(t)}}$ then reads

$$\nu_1\overset{\triangledown}{\overline{\mathbb{B}_{\kappa_{p(t)}}}} + \mu\left(\mathbb{B}_{\kappa_{p(t)}} - \mathbb{I}\right) = 2\tilde{\mu}\left(\Delta\operatorname{Tr}\mathbb{B}_{\kappa_{p(t)}}\right)\mathbb{B}_{\kappa_{p(t)}} + 2\frac{\mathrm{d}\tilde{\mu}}{\mathrm{d}\theta}\left[\left(\nabla\operatorname{Tr}\mathbb{B}_{\kappa_{p(t)}}\right)\bullet\nabla\theta\right]\mathbb{B}_{\kappa_{p(t)}}, \qquad (47)$$

see [**P6**] for details. Assuming that the material function $\tilde{\mu}$ is a constant, we see that equation (47) is close to the desired one—we have the Laplace operator on the right-hand side of (47). However the Laplace operator is acting on a scalar function, not on the full $\mathbb{B}_{\kappa_{p(t)}}$ tensor. A remedy for this drawback could be based on further adjustment of the Helmholtz free energy. One can, for example, think of using $\left|\nabla\mathbb{B}_{\kappa_{p(t)}}:\nabla\mathbb{B}_{\kappa_{p(t)}}\right|^2$ instead of $\left|\nabla\operatorname{Tr}\mathbb{B}_{\kappa_{p(t)}}\right|^2$, where we use the notation

$$\nabla\mathbb{B}_{\kappa_{p(t)}}:\nabla\mathbb{B}_{\kappa_{p(t)}} =_{\text{def}} \frac{\partial\mathrm{B}_{ij}}{\partial x_m}\frac{\partial\mathrm{B}_{ij}}{\partial x_m}. \qquad (48)$$

This would however lead to constitutive relations wherein the Cauchy stress tensor is not symmetric. Although such theories based on the concept of *couple stress* exist in continuum mechanics, see, for example, Hadjesfandiari et al. [2014] and references therein, we prefer, if possible, not to use them.

Summary 3: Incompressible Oldroyd-B model via Gibbs free energy

Specific Gibbs free energy:

$$g(\theta, \mathbb{S}_{\kappa_{p(t)}}) =_{\mathrm{def}} g_{\mathrm{thermal}}(\theta) + \frac{\mu(\theta)}{2\rho} \mathrm{Tr}\left(\frac{\rho}{\mu(\theta)} \mathbb{S}_{\kappa_{p(t)}} - \left[\frac{\rho}{\mu(\theta)} \mathbb{S}_{\kappa_{p(t)}} + \mathbb{I} \right] \ln\left[\frac{\rho}{\mu(\theta)} \mathbb{S}_{\kappa_{p(t)}} + \mathbb{I} \right] \right)$$

$$g_{\mathrm{thermal}}(\theta) =_{\mathrm{def}} -c_{\mathrm{V,ref}}\theta\left(\ln\frac{\theta}{\theta_{\mathrm{ref}}} - 1 \right)$$

Reduced stress (notation):

$$\mathbb{S}_{\kappa_{p(t)}} =_{\mathrm{def}} \frac{\mathbb{T}_{\kappa_{p(t)}}}{\rho}$$

Entropy production:

$$\xi = \frac{1}{\theta}\left\{ 2\nu\mathbb{D}_\delta : \mathbb{D}_\delta + \frac{1}{2\nu_1}\mathbb{T}_{\kappa_{p(t)}}\left(\frac{\mathbb{T}_{\kappa_{p(t)}}}{\mu(\theta)} + \mathbb{I} \right)^{-1} : \mathbb{T}_{\kappa_{p(t)}} \right\} + \kappa\frac{\nabla\theta \bullet \nabla\theta}{\theta^2}$$

Material parameters: $c_{\mathrm{V,ref}}$ specific heat at constant volume – positive constant; $\mu(\theta)$ shear modulus – nonnegative function, typically proportional to θ; ν, ν_1 viscosity – nonnegative functions of the primitive variables, typically constants; κ thermal conductivity – nonnegative function of the primitive variables, typically constant

Evolution equations (mechanical variables p, $\boldsymbol{v}$, $\mathbb{T}_{\kappa_{p(t)}}$ and thermal variable θ):

$$\mathrm{div}\,\boldsymbol{v} = 0$$

$$\rho\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = \mathrm{div}\,\mathbb{T} + \rho\boldsymbol{b}$$

$$\nu_1\overset{\triangledown}{\overline{\left(\frac{\mathbb{T}_{\kappa_{p(t)}}}{\mu(\theta)} \right)}} + \mathbb{T}_{\kappa_{p(t)}} = 2\nu_1\mathbb{D}$$

$$-\rho\theta\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial g}{\partial\theta}(\theta, \mathbb{S}_{\kappa_{p(t)}}) \right) = \mathrm{div}\,(\kappa\theta) + 2\nu\mathbb{D}_\delta : \mathbb{D}_\delta + \frac{1}{2\nu_1}\mathbb{T}_{\kappa_{p(t)}}\left(\frac{\mathbb{T}_{\kappa_{p(t)}}}{\mu(\theta)} + \mathbb{I} \right)^{-1} : \mathbb{T}_{\kappa_{p(t)}}$$

Cauchy stress tensor:

$$\mathbb{T} = -p\mathbb{I} + 2\nu\mathbb{D}_\delta + \mathbb{T}_{\kappa_{p(t)}, \delta}$$

Thermodynamical relations:

$$\mathbb{H}_{\kappa_{p(t)}} = -\frac{\partial g}{\partial\mathbb{S}_{\kappa_{p(t)}}}(\theta, \mathbb{S}_{\kappa_{p(t)}})$$

$$\eta = -\frac{\partial g}{\partial\theta}(\theta, \mathbb{S}_{\kappa_{p(t)}})$$

Left Cauchy–Green tensor $\mathbb{B}_{\kappa_{p(t)}}$ and Hencky strain tensor $\mathbb{H}_{\kappa_{p(t)}}$ associated to the elastic response:

$$\mathbb{B}_{\kappa_{p(t)}} = \mathrm{e}^{2\mathbb{H}_{\kappa_{p(t)}}}$$

The second option is to interpret the stress diffusion term as a consequence of a non-standard entropy production mechanism. This is in principle consistent with the microscopic interpretation of the stress diffusion term in dilute polymeric fluids—here the term originates from Brownian motion of the centre of mass of polymeric chains. If we fix the entropy production as

$$\xi =_{\mathrm{def}} \frac{1}{\theta}\left\{ \frac{2\nu + 3\lambda}{3}\left(\mathrm{div}\,\boldsymbol{v}\right)^2 + 2\nu\mathbb{D}_\delta : \mathbb{D}_\delta + \frac{\mu^2}{2\nu_1}\left(\mathrm{Tr}\,\mathbb{B}_{\kappa_{p(t)}} + \mathrm{Tr}\,\mathbb{B}_{\kappa_{p(t)}}^{-1} - 6 \right) + \frac{\mu\tilde{\mu}(\theta)}{2\nu_1}\nabla\mathbb{B}_{\kappa_{p(t)}} : \nabla\mathbb{B}_{\kappa_{p(t)}} \right\} + \frac{\kappa\left|\nabla\theta\right|^2}{\theta^2},$$

$$(49)$$

then we get the evolution equation for $\mathbb{B}_{\kappa_{p(t)}}$ in the form

$$\nu_1 \overline{\mathbb{B}_{\kappa_{p(t)}}^{\triangledown}} = -\mu \left(\mathbb{B}_{\kappa_{p(t)}} - \mathbb{I} \right) + \frac{1}{2} \left[\operatorname{div} \left(\tilde{\mu} \nabla \mathbb{B}_{\kappa_{p(t)}} \right) \mathbb{B}_{\kappa_{p(t)}} + \mathbb{B}_{\kappa_{p(t)}} \operatorname{div} \left(\tilde{\mu} \nabla \mathbb{B}_{\kappa_{p(t)}} \right) \right]. \tag{50}$$

This gives us the desired Laplace operator applied on the full $\mathbb{B}_{\kappa_{p(t)}}$ tensor, see [**P6**] for details. We note that the key concept that allows us to go from (49) to (50) is, besides the identification of the *entropy production*, also the proper identification of the *entropy flux* $\boldsymbol{j}_\eta$.

Careful analysis[2] then reveals that more elaborate choice of the entropy production

$$\widetilde{\xi} =_{\text{def}} \frac{1}{\theta} \left\{ 2\nu \mathbb{D}_\delta : \mathbb{D}_\delta + \frac{\mu^2}{2\nu_1} \left(\operatorname{Tr} \mathbb{B}_{\kappa_{p(t)}} + \operatorname{Tr} \mathbb{B}_{\kappa_{p(t)}}^{-1} - 6 \right) \right\}$$

$$+ \frac{1}{\theta} \left\{ 2 \frac{\mu\tilde{\mu}}{\nu} \operatorname{Tr} \left[\operatorname{Sym} \left(\mathbb{B}_{\kappa_{p(t)}}^{-\frac{1}{2}} \left(\nabla \mathbb{B}_{\kappa_{p(t)}}^{\frac{1}{2}} \right) \right) \bullet \operatorname{Sym} \left(\mathbb{B}_{\kappa_{p(t)}}^{-\frac{1}{2}} \left(\nabla \mathbb{B}_{\kappa_{p(t)}}^{\frac{1}{2}} \right) \right) \right] \right\} + \frac{\kappa \left| \nabla \theta \right|^2}{\theta^2}, \tag{51}$$

where $\operatorname{Sym}()$ denotes the symmetric part of the corresponding tensor, then leads to the evolution equation precisely in the desired form with the Laplace operator acting on $\mathbb{B}_{\kappa_{p(t)}}$,

$$\nu_1 \overline{\mathbb{B}_{\kappa_{p(t)}}^{\triangledown}} = -\mu \left(\mathbb{B}_{\kappa_{p(t)}} - \mathbb{I} \right) + \operatorname{div} \left(\tilde{\mu} \nabla \mathbb{B}_{\kappa_{p(t)}} \right). \tag{52}$$

While [**P6**] is focused on a diffusive variant of Oldroyd-B model, the follow-up work Dostalík et al. [2019a] we then investigate other popular viscoelastic rate-type models such as Giesekus, FENE-P, Johnson–Segalman, Phan-Thien–Tanner and Bautista–Manero–Puig models. We emphasise that in Dostalík et al. [2019a] we also work with other objective tensorial rates beyond the upper convected derivative (3). (An updated version posted on arXiv, arXiv:1902.07983, corrects some misprints in the published paper.) The analysis of thermodynamic background of viscoelastic rate-type models with stress diffusion has been then partially used in mathematical analysis of the corresponding governing equations, see Bulíček et al. [2018, 2021] and Bathory et al. [2021].

4. Viscoelastic micro-macro models

So far we have been dealing with purely phenomenological models, but the assumption that the material is fully characterised by its energy storage ability and its entropy production ability applies in microscopic setting as well, see, for example, our work Dostalík et al. [2020].

Without going into details, we recall that the standard micro-macro viscoelastic rate-type model for a compressible dilute polymeric liquid, see Öttinger and Grmela [1997], reads

$$\frac{\mathrm{d}\rho_{\text{s}}}{\mathrm{d}t} + \rho_{\text{s}} \operatorname{div}_{\boldsymbol{x}} \boldsymbol{v} = 0, \tag{53a}$$

$$\rho_{\text{s}} \frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = \operatorname{div}_{\boldsymbol{x}} \mathbb{T} + \rho_{\text{s}} \boldsymbol{b}, \tag{53b}$$

$$\frac{\partial \varphi}{\partial t} + \operatorname{div}_{\boldsymbol{x}} \left(\boldsymbol{v}\varphi - \frac{k_{\text{B}}\theta_{\text{s}}}{2\zeta} \nabla_{\boldsymbol{x}} \varphi \right) + \operatorname{div}_{\boldsymbol{q}} \left((\nabla_{\boldsymbol{x}} \boldsymbol{v}) \boldsymbol{q}\varphi - \frac{2\boldsymbol{F}}{\zeta} \varphi - \frac{2k_{\text{B}}\theta_{\text{s}}}{\zeta} \nabla_{\boldsymbol{q}} \varphi \right) = 0, \tag{53c}$$

and

$$\rho_{\text{s}} c_{\text{V,s}} \frac{\mathrm{d}\theta_{\text{s}}}{\mathrm{d}t} = -\theta_{\text{s}} \frac{\partial p_{\text{th,s}}}{\partial \theta_{\text{s}}} \operatorname{div}_{\boldsymbol{x}} \boldsymbol{v} + \operatorname{div}_{\boldsymbol{x}} \left(\kappa \nabla_{\boldsymbol{x}} \theta_{\text{s}} \right) + \lambda \left(\operatorname{div}_{\boldsymbol{x}} \boldsymbol{v} \right)^2 + 2\nu \mathbb{D} : \mathbb{D} - 2k_{\text{B}}\theta_{\text{s}} n_{\text{p}} \operatorname{div}_{\boldsymbol{x}} \boldsymbol{v}$$

$$+ \left[\int_D \left(\nabla_{\boldsymbol{q}} \frac{\theta_{\text{s}}}{\theta_{\text{ref}}} U_\eta \right) \otimes \boldsymbol{q}\varphi \, \mathrm{d}\boldsymbol{q} \right] : \mathbb{D} + \frac{2}{\zeta} \int_D \left(\nabla_{\boldsymbol{q}} U_e \right) \bullet \nabla_{\boldsymbol{q}} \left(U_e + \frac{\theta_{\text{s}}}{\theta_{\text{ref}}} U_\eta \right) \mathrm{d}\boldsymbol{q} - \frac{2k_{\text{B}}\theta_{\text{s}}}{\zeta} \int_D \left[\Delta_{\boldsymbol{q}} U_e \right] \varphi \, \mathrm{d}\boldsymbol{q}, \tag{53d}$$

where the unknown fields are the *velocity field* $\boldsymbol{v}$, solvent density ρ_{s}, solvent temperature θ_{s} and probability distribution function φ. (For details concerning the notation and physical interpretation of the variables please see Dostalík et al. [2020].) The constitutive relation for the dumbbell spring force $\boldsymbol{F}$ is given via the specification of potentials U_e and U_η,

$$\boldsymbol{F} =_{\text{def}} \nabla_{\boldsymbol{q}} \left[U_e \left(\frac{1}{2} \left| \frac{\boldsymbol{q}}{q_{\text{ref}}} \right|^2 \right) + \frac{\theta_{\text{s}}}{\theta_{\text{ref}}} U_\eta \left(\frac{1}{2} \left| \frac{\boldsymbol{q}}{q_{\text{ref}}} \right|^2 \right) \right], \tag{53e}$$

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[2]Miroslav Bulíček, personal communication.

while the Cauchy stress tensor $\mathbb{T}$ is given by the formula

$$\mathbb{T} =_{\text{def}} -p_{\text{th,s}}\mathbb{I} + \lambda\left(\text{div}_{\boldsymbol{x}}\boldsymbol{v}\right)\mathbb{I} + 2\nu\mathbb{D} - 2k_{\text{B}}\theta_{\text{s}}n_{\text{p}}\mathbb{I} + \int_{D}\boldsymbol{F}\otimes\boldsymbol{q}\varphi\,\mathrm{d}\boldsymbol{q}, \tag{53f}$$

$$p_{\text{th,s}} =_{\text{def}} \frac{c_{\text{V,s}}\left(\gamma - 1\right)\rho_{\text{s}}\theta_{\text{s}}}{1 - b\rho_{\text{s}}} - p_{\infty}, \tag{53g}$$

where we have used the Nobel–Abel stiffened gas equation of state, Le Métayer and Saurel [2016], Chiapolino and Saurel [2018].

The Helmhotz free energy behind the governing equations can be identified, see Dostalík et al. [2020], and it is given by the formulae

$$\psi(\theta_{\text{s}}, \rho_{\text{s}}, \varphi) =_{\text{def}} \psi_{\text{s}}(\theta_{\text{s}}, \rho_{\text{s}}) + \frac{1}{\rho_{\text{s}}}\int_{D}U_{e}\left(\frac{1}{2}\left|\frac{\boldsymbol{q}}{q_{\text{ref}}}\right|^{2}\right)\varphi\,\mathrm{d}\boldsymbol{q} + \frac{k_{\text{B}}\theta_{\text{s}}}{\rho_{\text{s}}}\int_{D}\left(\frac{U_{\eta}\left(\frac{1}{2}\left|\frac{\boldsymbol{q}}{q_{\text{ref}}}\right|^{2}\right)}{k_{\text{B}}\theta_{\text{ref}}}\varphi + \varphi\ln\frac{\varphi}{K}\right)\mathrm{d}\boldsymbol{q} \tag{54a}$$

and

$$\psi_{\text{s}}(\theta_{\text{s}}, \rho_{\text{s}}) =_{\text{def}} -c_{\text{V,s}}\theta_{\text{s}}\left[\ln\left(\frac{\theta_{\text{s}}}{\theta_{\text{s,ref}}}\right) - 1\right] - c_{\text{V,s}}\theta_{\text{s}}\left(1 - \gamma\right)\ln\left[\frac{c_{\text{V,s}}\left(\gamma - 1\right)\rho_{\text{s}}}{1 - b\rho_{\text{s}}}\frac{\theta_{\text{s,ref}}}{p_{\text{ref}}}\right]$$
$$-q'\theta_{\text{s}} + \left(\frac{1}{\rho_{\text{s}}} - b\right)p_{\infty} + q, \tag{54b}$$

where U_{η} and U_{e} are some given spring potentials. The corresponding entropy production reads

$$\xi = \frac{1}{\theta_{\text{s}}}\left(2\nu\mathbb{D}_{\delta} : \mathbb{D}_{\delta} + \tilde{\lambda}\left(\text{div}_{\boldsymbol{x}}\boldsymbol{v}\right)^{2}\right)$$
$$+ \frac{2}{\theta_{\text{s}}\zeta}\int_{D}\frac{1}{\varphi}\left|\left(\frac{\mathrm{d}U_{e}}{\mathrm{d}s}\bigg|_{s=\frac{1}{2}\left|\frac{\boldsymbol{q}}{q_{\text{ref}}}\right|^{2}} + \frac{\theta_{\text{s}}}{\theta_{\text{ref}}}\frac{\mathrm{d}U_{\eta}}{\mathrm{d}s}\bigg|_{s=\frac{1}{2}\left|\frac{\boldsymbol{q}}{q_{\text{ref}}}\right|^{2}}\right)\frac{\boldsymbol{q}}{q_{\text{ref}}^{2}}\varphi + k_{\text{B}}\theta_{\text{s}}\nabla_{\boldsymbol{q}}\varphi\right|^{2}\mathrm{d}\boldsymbol{q}$$
$$+ \frac{k_{\text{B}}^{2}\theta_{\text{s}}}{2\zeta}\int_{D}\frac{1}{\varphi}\left|\nabla_{\boldsymbol{x}}\varphi\right|^{2}\mathrm{d}\boldsymbol{q} + \kappa\frac{\left|\nabla_{\boldsymbol{x}}\theta_{\text{s}}\right|^{2}}{\theta_{\text{s}}^{2}}, \tag{55}$$

see Dostalík et al. [2020] for details.

The point of this short excursion is to add a final argument to the claim that the viscoelastic rate-type models can be quite complex and that they are typically coupled—thermal variables influence the evolution of mechanical variables and *vice versa*. Consequently, analysis of qualitative behaviour predicted by the governing equations (53) or by governing equations shown in Summary 2 and similar ones, can be quite challenging. Fortunately, thermodynamics offers us a helping hand. The knowledge of thermodynamic background of the models can be gainfully exploited, for example, in nonlinear stability analysis. Such an analysis is the subject of the last chapter.

CHAPTER 4

Stability

Having invested a lot of effort into development of thermodynamically consistent models for viscoelastic fluids, one can ask whether such an effort has been worth of it. In fact the viscoelastic rate-type models have been for a long time gainfully used without proper understanding of the underlying thermodynamic background. Thus our question [**Q4**] is *how to exploit thermodynamics in analysis of qualitative behaviour of solutions to the corresponding systems of nonlinear partial differential equations.* Our answer is that the effort invested in the development of thermodynamically consistent models pays off, amongst others, in *nonlinear stability analysis* of solutions to the corresponding nonlinear partial differential equations.

Parts of the following text are based on our recent review paper Dostalík and Průša [2022]. We have first dealt with the topic in [**P1**], while the general approach is then applied/tested in a purely mechanical context in [**P4**] and in a full thermo-mechanical setting in [**P2**] and [**P3**].

1. Concept of stability and related mathematical techniques and problems

The objective is to establish stability of a steady state in a system whose dynamics is governed by a differential equation. (In our case by a system of nonlinear partial differential equations.) Informally, the task is the following. If the system of governing equations has a steady solution $\widehat{\boldsymbol{W}}$, then we say that the solution is *asymptotically stable* provided that any solution $\boldsymbol{W}$ starting from a perturbed steady state remain close to the steady state (Lyapunov stability), and, furthermore, if

$$\left\|\widehat{\boldsymbol{W}} - \boldsymbol{W}\right\|_{\mathrm{st}} \xrightarrow{t \to +\infty} 0, \tag{56}$$

where $\|\cdot\|_{\mathrm{st}}$ is a norm, see Figure 1 for a sketch. The size of the initial perturbation can be restricted or unrestricted. In the former case one talks about *conditional stability*, while in the latter case when all perturbations are attracted to the steady state one talks about *unconditional stability*.
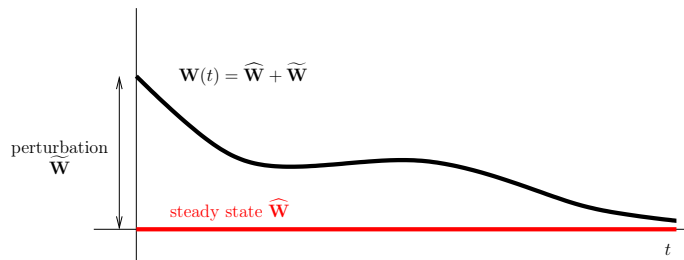
FIGURE 1. Concept of stability.

The standard tool for nonlinear stability analysis is the Lyapunov functional, see, for example, Henry [1981] for a discussion that applies to the infinite dimensional setting. We consider a system of governing equations in the form

$$\frac{\mathrm{d}\boldsymbol{W}}{\mathrm{d}t} = \boldsymbol{F}(\boldsymbol{W}), \tag{57}$$

where $\widehat{\boldsymbol{W}}$ is a steady state, that is $\boldsymbol{F}(\widehat{\boldsymbol{W}}) = \boldsymbol{0}$, and where $\|\cdot\|_{\mathrm{st}}$ denotes a norm on the underlying state space. We say that the functional $\mathcal{V}(\widetilde{\boldsymbol{W}}\|\widehat{\boldsymbol{W}})$ is a strict Lyapunov functional of the steady state $\widehat{\boldsymbol{W}}$ provided that:

(1) There exists a neighborhood of $\widehat{\boldsymbol{W}}$ such that the functional is bounded from below by a function f of the distance between the steady state $\widehat{\boldsymbol{W}}$ and the perturbation $\boldsymbol{W}$, that is

$$\mathcal{V}\left(\widetilde{\boldsymbol{W}}\,\|\,\widehat{\boldsymbol{W}}\right) \geq f\left(\left\|\widehat{\boldsymbol{W}} - \boldsymbol{W}\right\|_{\text{st}}\right), \tag{58a}$$

where f is a continuous strictly increasing function such that $f(0) = 0$ and $f(r) > 0$ whenever $r > 0$.

(2) The time derivative of $\mathcal{V}(\widetilde{\boldsymbol{W}}\,\|\,\widehat{\boldsymbol{W}})$ is negative and bounded from above by a function g of the distance between the steady state $\widehat{\boldsymbol{W}}$ and the perturbation $\boldsymbol{W}$, that is

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{V}\left(\widetilde{\boldsymbol{W}}\,\|\,\widehat{\boldsymbol{W}}\right) \leq -g\left(\left\|\widehat{\boldsymbol{W}} - \boldsymbol{W}\right\|_{\text{st}}\right), \tag{58b}$$

where g is a continuous strictly increasing function such that $g(0) = 0$ and $g(r) > 0$ whenever $r > 0$.

We note that the theorem can be rephrased in metric spaces as well.

If the given system of governing equations admits a strict Lyapunov functional near the state $\widehat{\boldsymbol{W}}$, then we know that the steady state $\widehat{\boldsymbol{W}}$ is conditionally asymptotically stable. This means that the solution $\boldsymbol{W} = \widetilde{\boldsymbol{W}} + \widehat{\boldsymbol{W}}$ that starts in the neighborhood of $\widehat{\boldsymbol{W}}$ satisfies

$$\left\|\widehat{\boldsymbol{W}} - \boldsymbol{W}\right\|_{\text{st}} \xrightarrow{t \to +\infty} 0. \tag{59}$$
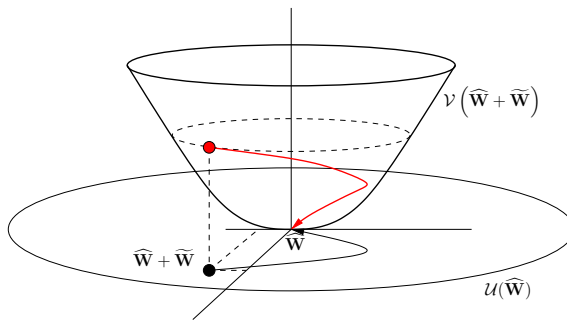

FIGURE 2. Lyapunov functional.

Consequently, the stability analysis boils down to the identification of a suitable Lyapunov functional. However, this is not easy. *The more complex the governing equations, the harder is to identify the suitable Lyapunov functional.* (Think for example about system of equations (53) for a dilute polymeric fluid—what is a suitable Lyapunov functional for such system?) In other words, the more complex the governing equations, the less likely is to succeed with *ad hoc* constructions of Lyapunov functional. A systematic approach to construction of Lyapunov functionals is needed, and here is the point where thermodynamics offers a helping hand.

Before we proceed with thermodynamically motivated construction of Lyapunov functionals, we point out some mathematical and physical issues we need to face. Mathematical issues are related to the fact that we work with partial differential equations, which means that we work in *infinite dimensional* state spaces. Physical issues are related to the fact that we need to carefully work with the *boundary conditions*, and that we need to work with fully coupled thermomechanical systems.

1.1. Mathematical issues. First, the choice of topology on the underlying state space is essential; it is not a matter of convenience as in the finite dimensional case. The reason is that in the infinite dimensional setting different norms are not in general equivalent as in the finite dimensional case. Consequently, the solution can be shown to be asymptotically stable using a particular choice of the norm/distance, but it might be unstable if one chooses a different norm/distance; specific examples are given in Flavin and Rionero [1995].

Another typical problem dwells in the fact that if we know that a function tends to zero, the same is not necessarily true for its derivative/gradient. (The standard counterexample is the function $f(n, x) = \frac{1}{n}\sin\left(n^2 x\right)$ that for arbitrary x satisfies $\lim_{n \to +\infty} f(n, x) = 0$, but $\lim_{n \to +\infty} \frac{\mathrm{d}f}{\mathrm{d}x}(n, x) \neq$

0. The limit of the derivative even does not exist.) However, the argument "if a function vanishes, then its gradient must vanish as well," is frequently used in various non-rigorous physical works. Albeit such a behaviour can be expected, it is not granted *a priori*; such a behaviour must be inferred from the governing equations.

Finally, various theorems referring to the concept of Lyapunov functional, for example the *LaSalle invariance principle*, typically hold in the *infinite* dimensional setting only under stronger assumptions than in the *finite* dimensional setting, for details see, for example, Henry [1981] or Šilhavý [1997]. Naturally, the stronger assumptions are more difficult to work with. For instructive counterexamples showing peculiarities of the infinite dimensional setting we refer the reader to Zwart [2015].

1.2. Physical issues. At first glance, it may seem that the construction of physically motivated Lyapunov functionals is straightforward. For example, if we deal with a spring–mass system with damping, see Figure 3, then the governing equation for the spring elongation x reads

$$m\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -b\frac{\mathrm{d}x}{\mathrm{d}t} - k(x - x_{\mathrm{eq}}),\tag{60}$$

where x_{eq} denotes the equilibrium length of the spring, see Figure 3, and m, k and b are constants (mass, spring stiffness, damping coefficient). The equilibrium length of the spring x_{eq} is the steady solution to (60), and using the notation introduced above we can thus identify $\boldsymbol{W} =_{\mathrm{def}} x$ and $\widehat{\boldsymbol{W}} =_{\mathrm{def}} x_{\mathrm{eq}}$. Using (60) it is easy to conclude that the evolution equation for the perturbation $\widetilde{x}$ reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\underbrace{\frac{1}{2}m\left(\frac{\mathrm{d}\widetilde{x}}{\mathrm{d}t}\right)^2}_{\text{kinetic energy}} + \underbrace{\frac{1}{2}k\widetilde{x}^2}_{\text{elastic stored energy}}\right] = \underbrace{-b\left(\frac{\mathrm{d}\widetilde{x}}{\mathrm{d}t}\right)^2}_{\text{dissipation}}.\tag{61}$$

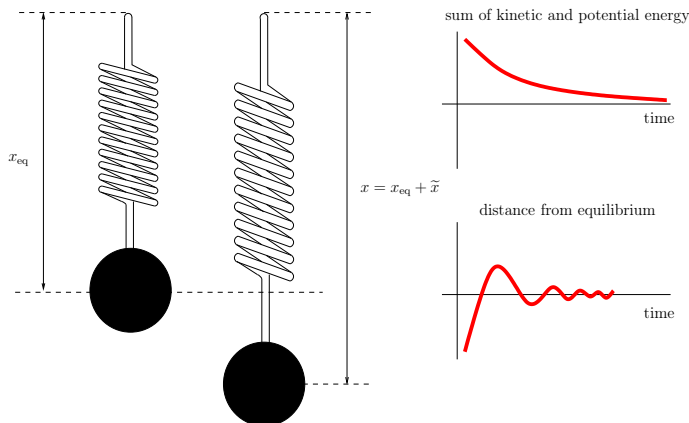From (61) it follows $\widetilde{x} \to 0$ as $t \to +\infty$.

FIGURE 3. Damped spring and its long-term dynamics.

In this case the sum of the kinetic energy and the elastic stored energy decreases—it is lost due to the dissipation. In virtue of this observation, we can immediately identify the Lyapunov function and establish the desired stability result. At this point one might think that the identification of the mechanical energy and the dissipation would suffice even in the continuum mechanics setting.

The situation is however much more challenging in the continuum mechanics setting. First, in a coupled thermo-mechanical system the net total energy is typically conserved (thermodynamically isolated system) or its time derivative is *a priori* unknown (thermodynamically open systems). The stability of a steady state is not related to the decay of net total energy, instead we are dealing with *reorganisation of the energy distribution in space*. Second, the solution of the corresponding system of partial differential equations *depends on the choice of boundary conditions*, and the same holds for stability analysis. In other words, the boundary conditions are as important as the governing equations themselves.

2. Construction of Lyapunov type functionals

The systematic construction of Lyapunov type functionals differs for *thermodynamically open systems* and *thermodynamically isolated systems*, see [**P1**]. The case of thermodynamically isolated systems is simpler, since there is no need to work with *fluxes through the boundary* of the system.

2.1. Thermodynamically isolated systems.

2.1.1. *Expected qualitative behaviour.* Thermodynamically isolated systems are not allowed to interact with the outside environment, see Figure 4 for a sketch. If the system of interest is a *dissipative* one, then the expected dynamical behaviour is pretty boring. The spatially homogeneous steady state is expected to be stationary (zero macroscopic velocity field) and stable with respect to *any* perturbation. The ambition is to *prove* that this actually happens for *any* initial perturbation. In particular, one can not focus on "infinitesimal" perturbations described by the linearisation of the governing equations—a truly nonlinear theory is needed.
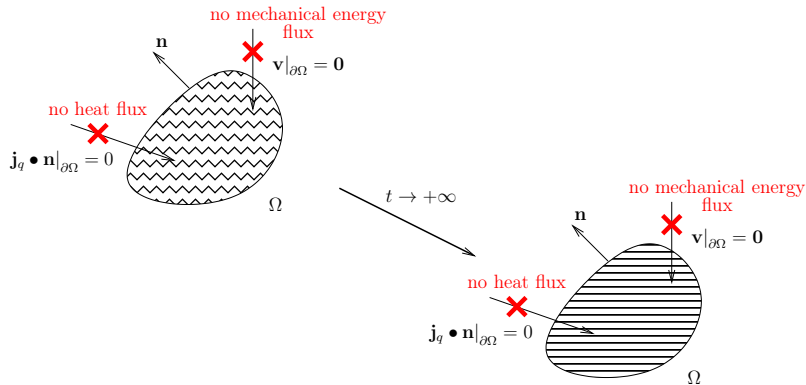

FIGURE 4. Thermodynamically isolated system.

We note that this goal can not be achieved using the frequently referred approach proposed by Glansdorff and Prigogine [1971]. (Albeit the approach is clearly beneficial provided that one is interested in necessary conditions for *in*stability. The comment applies to the open systems as well, see the discussion below.) Indeed, Glansdorff and Prigogine [1971] propose to track the time evolution of perturbations using a functional that involves the *second variation* of the net entropy functional, hence the perturbations are essentially measured by the means of a quantity "quadratic" in perturbations. This is clearly insufficient in a fully nonlinear setting.

2.1.2. *Lyapunov type functional.* The path to the fully nonlinear setting starts with the famous statement by Clausius [1865]: "The energy of the world is constant. The entropy of the world strives to a maximum." If the statement is understood in the sense that the net entropy in an isolated system must increase in time, and that all other relevant net quantities such as the energy and the total mass must be conserved, then the statement suggests that the functional

$$\mathcal{V}_{\mathrm{eq}} =_{\mathrm{def}} -S + \lambda_1 \left(E_{\mathrm{tot}} - \widehat{E_{\mathrm{tot}}} \right) + \lambda_2 \int_\Omega \left(\rho - \widehat{\rho} \right) \mathrm{dv} \tag{62}$$

might be of interest regarding the monitoring of the approach to the target stationary state. Here the symbol S denotes the net entropy,

$$S =_{\mathrm{def}} \int_\Omega \rho \eta \, \mathrm{dv}, \tag{63}$$

and the symbol E_{tot} denotes the net total energy

$$E_{\mathrm{tot}} =_{\mathrm{def}} \int_\Omega \left(\frac{1}{2} \rho \left| \boldsymbol{v} \right|^2 + \rho e \right) \mathrm{dv} \tag{64}$$

at the current state, and $\widehat{E_{\mathrm{tot}}}$ denotes the net total energy at the stationary spatially homogeneous stationary state, $\widehat{E_{\mathrm{tot}}} = \int_\Omega \widehat{\rho e}\, \mathrm{dv}$ respectively, and Ω is the domain of interest. Finally, symbols λ_1 and λ_2 denote appropriately chosen Lagrange multipliers, see Section 2.1.3 below for detailed discussion.

Depending on the particular system of interest *other constraints must be added on the right-hand side* of (62). For example for dilute polymeric fluids one has to enforce also conservation of the number of polymeric chains, that is

$$\mathcal{V}_{\text{meq}} = -S + \lambda_1 \left(E_{\text{tot}} - \widehat{E_{\text{tot}}} \right) + \lambda_2 \int_\Omega \left(\rho_{\text{s}} - \widehat{\rho_{\text{s}}} \right) \mathrm{dv} + \lambda_3 \int_\Omega \left(n_{\text{p}} - \widehat{n_{\text{p}}} \right) \mathrm{dv}, \tag{65}$$

where λ_3 denotes a new Lagrange multiplier and n_{p} denotes the current density of polymeric chains and $\widehat{n_{\text{p}}}$ denotes the steady state density of polymeric chains.

The approach based on (62) in principle leads to a functional that is *decreasing in time* and nonnegative, and that vanishes if and only if the perturbation vanishes. Indeed, the time derivative of the functional (62) reads

$$\frac{\mathrm{d}\mathcal{V}_{\text{meq}}}{\mathrm{d}t} = -\frac{\mathrm{d}S}{\mathrm{d}t} = -\int_\Omega \xi \,\mathrm{dv} \le 0, \tag{66}$$

where we have used the fact the net total energy and mass in an isolated system are conserved, and that the definition of net total entropy (63) in virtue of generic entropy evolution equation (43) and the *absence of entropy flux $\boldsymbol{j}_\eta$ through the boundary* imply that

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \int_\Omega \xi \,\mathrm{dv} - \int_{\partial\Omega} \boldsymbol{j}_\eta \bullet \boldsymbol{n} \,\mathrm{ds} = \int_\Omega \xi \,\mathrm{dv}, \tag{67}$$

where the entropy production ξ is a nonnegative quantity.

The guaranteed nonpositivity of the time derivative $\frac{\mathrm{d}\mathcal{V}_{\text{meq}}}{\mathrm{d}t}$ and the nonnegativity of the functional $\mathcal{V}_{\text{meq}}$ make the functional an ideal *candidate* for the Lyapunov functional for the nonlinear stability analysis. However, the relation of the functional to a *suitable norm/metric* on the corresponding state space in the sense of inequalities (58) might not be clear, hence we prefer to denote functionals of type (62) only as *Lyapunov type* functionals.

In continuum thermodynamics setting the idea to use functionals of type (62) in nonlinear stability analysis was introduced by Coleman and Greenberg [1967], Coleman [1970] and Gurtin [1973, 1975], though its origins can be traced back to Duhem [1911].

2.1.3. *Identification of Lagrange multipliers in Lyapunov type functional.* The Lagrange multipliers in (62) can be identified via solution of a constrained maximisation problem, see [**P1**] for details. In [**P1**] we however deal with an incompressible material only, the treatment of a compressible material is discussed below.

We want the net entropy S at the stationary state to be maximal subject to the corresponding constraints. The auxilliary functional for the constrained maximisation problems is, up to the sign, the functional (62). If we use the definitions of the net entropy and the net total energy, we get the auxilliary functional in the form

$$\mathcal{L}_{\lambda_1,\lambda_2} =_{\text{def}} \int_\Omega \rho\eta \,\mathrm{dv} - \lambda_1 \int_\Omega \left(\frac{1}{2}\rho |\boldsymbol{v}|^2 + \rho e - \widehat{\rho e} \right) \mathrm{dv} - \lambda_2 \int_\Omega (\rho - \widehat{\rho}) \,\mathrm{dv}. \tag{68}$$

The stationary spatially homogeneous state $\widehat{\rho}$, $\widehat{\theta}$ and $\widehat{\boldsymbol{v}} = \boldsymbol{0}$ is a solution to the maximisation problem provided that the Gâteaux derivative[1] of auxilliary functional (68) at point $\widehat{\rho}$, $\widehat{\theta}$ and $\widehat{\boldsymbol{v}}$ vanishes in every admissible direction $\widetilde{\rho}$, $\widetilde{\theta}$ and $\widetilde{\boldsymbol{v}}$. Now we evaluate the Gâteaux derivative in two different descriptions, which allows us to identify the multipliers λ_1 and λ_2. The idea is the following. The fact that the net entropy is at maximum value must be true no matter whether our primitive variables are the temperature and the density, or the temperature and the pressure and so forth; consequently *we can conveniently switch between various descriptions in order to get the desired piece of information.*

First, we interpret the entropy and the internal energy as functions of the density ρ and the temperature θ. The formula for the Gâteaux derivative at point $\widehat{\rho}$, $\widehat{\theta}$ and $\widehat{\boldsymbol{v}}$ in the direction $\widetilde{\theta}$, $\widetilde{\rho}$

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[1]We recall that the Gâteaux derivative $\mathrm{D}\mathcal{M}(\boldsymbol{x})[\boldsymbol{y}]$ of a functional $\mathcal{M}$ at point $\boldsymbol{x}$ in the direction $\boldsymbol{y}$ is defined as $\mathrm{D}\mathcal{M}(\boldsymbol{x})[\boldsymbol{y}] =_{\text{def}} \lim_{s\to 0} \frac{\mathcal{M}(\boldsymbol{x}+s\boldsymbol{y})-\mathcal{M}(\boldsymbol{x})}{s}$ which is tantamount to $\mathrm{D}\mathcal{M}(\boldsymbol{x})[\boldsymbol{y}] =_{\text{def}} \frac{\mathrm{d}}{\mathrm{d}s}\mathcal{M}(\boldsymbol{x}+s\boldsymbol{y})\big|_{s=0}$. If it is necessary to emphasize the variable against which we differentiate, we also write $\mathrm{D}_{\boldsymbol{x}}\mathcal{M}(\boldsymbol{x})[\boldsymbol{y}]$ instead of $\mathrm{D}\mathcal{M}(\boldsymbol{x})[\boldsymbol{y}]$.

and $\widetilde{v}$ reads

$$\mathrm{D}\mathcal{L}_{\lambda_1,\lambda_2}(\widehat{\theta},\widehat{\rho},\mathbf{0})[\widetilde{\theta},\widetilde{\rho},\widetilde{v}] =$$

$$\frac{\mathrm{d}}{\mathrm{d}s}\left\{\int_\Omega (\widehat{\rho}+s\widetilde{\rho})\,\eta(\widehat{\rho}+s\widetilde{\rho},\widehat{\theta}+s\widetilde{\theta})\,\mathrm{d}v - \lambda_1 \int_\Omega \left(\frac{1}{2}(\widehat{\rho}+s\widetilde{\rho})\,|s\widetilde{v}|^2 + \rho e(\widehat{\rho}+s\widetilde{\rho},\widehat{\theta}+s\widetilde{\theta}) - \widehat{\rho e}(\widehat{\rho},\widehat{\theta})\right)\mathrm{d}v\right.$$

$$\left.-\lambda_2 \int_\Omega (\widehat{\rho}+s\widetilde{\rho}-\widehat{\rho})\,\mathrm{d}v\right\}\bigg|_{s=0}, \quad (69)$$

which with a slight abuse of notation yields

$$\mathrm{D}\mathcal{L}_{\lambda_1,\lambda_2}(\widehat{\theta},\widehat{\rho},\mathbf{0})[\widetilde{\theta},\widetilde{\rho},\widetilde{v}] = \int_\Omega \widehat{\rho}\left(\frac{\partial\eta(\widehat{\rho},\widehat{\theta})}{\partial\widehat{\theta}} - \lambda_1 \frac{\partial e(\widehat{\rho},\widehat{\theta})}{\partial\widehat{\theta}}\right)\widetilde{\theta}\,\mathrm{d}v, \quad (70)$$

where we have used the fact that $\int_\Omega \widetilde{\rho}\,\mathrm{d}v = 0$, which is a consequence of the mass conservation constraint. (Recall that the stationary state is spatially homogeneous, hence $\widehat{\theta}$ and $\widehat{\rho}$ are constants. The abuse of notation is about using $\frac{\partial\eta(\widehat{\rho},\widehat{\theta})}{\partial\widehat{\theta}}$ as an abbreviation for $\frac{\partial\eta(\rho,\theta)}{\partial\theta}\big|_{(\rho,\theta)=(\widehat{\rho},\widehat{\theta})}$.) Using standard thermodynamic identities

$$\frac{\partial\widehat{\eta}(\widehat{\theta},\widehat{\rho})}{\partial\widehat{\theta}} = \frac{c_\mathrm{V}(\widehat{\rho},\widehat{\theta})}{\widehat{\theta}}, \quad (71\mathrm{a})$$

$$\frac{\partial\widehat{e}(\widehat{\theta},\widehat{\rho})}{\partial\widehat{\theta}} = c_\mathrm{V}(\widehat{\rho},\widehat{\theta}), \quad (71\mathrm{b})$$

where c_V denotes the specific heat at constant volume, we see that (70) reduces to

$$\mathrm{D}\mathcal{L}_{\lambda_1,\lambda_2}(\widehat{\theta},\widehat{\rho},\mathbf{0})[\widetilde{\theta},\widetilde{\rho},\widetilde{v}] = \int_\Omega \widehat{\rho}\left(\frac{1}{\widehat{\theta}}-\lambda_1\right)c_\mathrm{V}(\widehat{\rho},\widehat{\theta})\widetilde{\theta}\,\mathrm{d}v. \quad (72)$$

The Gâteaux derivative therefore vanishes for arbitrary $\widetilde{\theta}$ provided that we fix the Lagrange multiplier as

$$\lambda_1 = \frac{1}{\widehat{\theta}}. \quad (73)$$

The second Lagrange multiplier λ_2 is however still unidentified. In order to identify it, we need to switch to a different set of variables.

Now we interpret the entropy and the internal energy as functions of the density ρ and the thermodynamic pressure p_th. The formula for the Gâteaux derivative at point $\widehat{\rho}$, $\widehat{p_\mathrm{th}}$ and $\widehat{v}$ in the direction $\widetilde{\theta}$, $\widetilde{p_\mathrm{th}}$ and $\widetilde{v}$ reads

$$\mathrm{D}\mathcal{L}_{\lambda_1,\lambda_2}(\widehat{\theta},\widehat{p_\mathrm{th}},\mathbf{0})[\widetilde{\theta},\widetilde{p_\mathrm{th}},\widetilde{v}] = \frac{\mathrm{d}}{\mathrm{d}s}\left\{\int_\Omega \rho(\widehat{\theta}+s\widetilde{\theta},\widehat{p_\mathrm{th}}+s\widetilde{p_\mathrm{th}})\eta(\widehat{\theta}+s\widetilde{\theta},\widehat{p_\mathrm{th}}+s\widetilde{p_\mathrm{th}})\right.$$

$$\left.-\lambda_1 \int_\Omega \left(\frac{1}{2}\rho(\widehat{\theta}+s\widetilde{\theta},\widehat{p_\mathrm{th}}+s\widetilde{p_\mathrm{th}})\,|s\widetilde{v}|^2 + \rho(\widehat{\theta}+s\widetilde{\theta},\widehat{p_\mathrm{th}}+s\widetilde{p_\mathrm{th}})e(\widehat{\theta}+s\widetilde{\theta},\widehat{p_\mathrm{th}}+s\widetilde{p_\mathrm{th}})\right)\mathrm{d}v\right.$$

$$\left.-\lambda_2 \int_\Omega \rho(\widehat{\theta}+s\widetilde{\theta},\widehat{p_\mathrm{th}}+s\widetilde{p_\mathrm{th}})\,\mathrm{d}v\right\}\bigg|_{s=0}. \quad (74)$$

(The density is now interpreted as a function of the primitive variables—the temperature and the thermodynamic pressure.) Straightforward calculation reveals that

$$\mathrm{D}\mathcal{L}_{\lambda_1,\lambda_2}(\widehat{\theta},\widehat{p_\mathrm{th}},\mathbf{0})[\widetilde{\theta},\widetilde{p_\mathrm{th}},\widetilde{v}]$$

$$= \int_\Omega \left\{\frac{\partial\rho(\widehat{\theta},\widehat{p_\mathrm{th}})}{\partial\widehat{\theta}}(\widehat{\eta}-\lambda_1\widehat{e}) + \widehat{\rho}\left(\frac{\partial\eta(\widehat{\theta},\widehat{p_\mathrm{th}})}{\partial\widehat{\theta}} - \lambda_1\frac{\partial e(\widehat{\theta},\widehat{p_\mathrm{th}})}{\partial\widehat{\theta}}\right) - \lambda_2\frac{\partial\rho(\widehat{\theta},\widehat{p_\mathrm{th}})}{\partial\widehat{\theta}}\right\}\widetilde{\theta}\,\mathrm{d}v$$

$$+ \int_\Omega \left(\frac{\partial\rho(\widehat{\theta},\widehat{p_\mathrm{th}})}{\partial\widehat{p_\mathrm{th}}}(\widehat{\eta}-\lambda_1\widehat{e}) + \widehat{\rho}\left(\frac{\partial\eta(\widehat{\theta},\widehat{p_\mathrm{th}})}{\partial\widehat{p_\mathrm{th}}} - \lambda_1\frac{\partial e(\widehat{\theta},\widehat{p_\mathrm{th}})}{\partial\widehat{p_\mathrm{th}}}\right) - \lambda_2\frac{\partial\rho(\widehat{\theta},\widehat{p_\mathrm{th}})}{\partial\widehat{p_\mathrm{th}}}\right)\widetilde{p_\mathrm{th}}\,\mathrm{d}v, \quad (75)$$

where we denote $\widehat{\rho} = \rho(\widehat{\theta},\widehat{p_\mathrm{th}})$, $\widehat{\eta} = \eta(\widehat{\theta},\widehat{p_\mathrm{th}})$ and $\widehat{e} = e(\widehat{\theta},\widehat{p_\mathrm{th}})$ and where we have again slightly abused the notation.

Since we have already identified the Lagrange multiplier λ_1 as $\lambda_1 = \frac{1}{\widehat{\theta}}$ we see that

$$\widehat{\eta} - \lambda_1\widehat{e} = \widehat{\eta} - \frac{1}{\widehat{\theta}}\widehat{e} = -\widehat{\theta\psi} = 0 \quad (76)$$

provided that the Helmholtz free energy $\psi =_{\mathrm{def}} e - \theta\eta$ is calibrated in such a way that it vanishes at the stationary spatially homogeneous state. Furthermore, using standard thermodynamical identities

$$\frac{\partial \eta(\widehat{\theta}, \widehat{\rho})}{\partial \widehat{\rho}} = -\frac{1}{\widehat{\rho}^2} \frac{\partial p_{\mathrm{th}}(\widehat{\theta}, \widehat{\rho})}{\partial \widehat{\theta}}, \tag{77a}$$

$$-p_{\mathrm{th}}(\widehat{\theta}, \widehat{\rho}) + \widehat{\rho}^2 \frac{\partial e(\widehat{\theta}, \widehat{\rho})}{\partial \widehat{\rho}} = -\widehat{\theta} \frac{\partial p_{\mathrm{th}}(\widehat{\theta}, \widehat{\rho})}{\partial \widehat{\theta}} \tag{77b}$$

we see that

$$\widehat{\rho}\left(\frac{\partial \eta(\widehat{\theta}, \widehat{p_{\mathrm{th}}})}{\partial \widehat{p_{\mathrm{th}}}} - \lambda_1 \frac{\partial e(\widehat{\theta}, \widehat{p_{\mathrm{th}}})}{\partial \widehat{p_{\mathrm{th}}}}\right) - \lambda_2 \frac{\partial \rho(\widehat{\theta}, \widehat{p_{\mathrm{th}}})}{\partial \widehat{p_{\mathrm{th}}}} = \widehat{\rho}\left(\frac{\partial \eta(\widehat{\theta}, \widehat{\rho})}{\partial \widehat{\rho}} - \lambda_1 \frac{\partial e(\widehat{\theta}, \widehat{\rho})}{\partial \widehat{\rho}}\right) \frac{\partial \rho(\widehat{\theta}, \widehat{p_{\mathrm{th}}})}{\partial \widehat{p_{\mathrm{th}}}} - \lambda_2 \frac{\partial \rho(\widehat{\theta}, \widehat{p_{\mathrm{th}}})}{\partial \widehat{p_{\mathrm{th}}}}$$

$$= \left(-\frac{\widehat{p_{\mathrm{th}}}}{\widehat{\rho}\widehat{\theta}} + \lambda_2\right) \frac{\partial \rho(\widehat{\theta}, \widehat{p_{\mathrm{th}}})}{\partial \widehat{p_{\mathrm{th}}}}, \tag{78}$$

where we have also used the formula (73) for the Lagrange multiplier λ_1. Observations (78) and (76) then allow us to rewrite the formula (75) for the Gâteaux derivative as

$$\mathrm{D}\mathcal{L}_{\lambda_1, \lambda_2}(\widehat{\theta}, \widehat{p_{\mathrm{th}}}, \mathbf{0})[\widetilde{\theta}, \widetilde{p_{\mathrm{th}}}, \widetilde{\boldsymbol{v}}] = \int_{\Omega} \left\{\widehat{\rho}\left(\frac{\partial \eta(\widehat{\theta}, \widehat{p_{\mathrm{th}}})}{\partial \widehat{\theta}} - \lambda_1 \frac{\partial e(\widehat{\theta}, \widehat{p_{\mathrm{th}}})}{\partial \widehat{\theta}}\right) - \lambda_2 \frac{\partial \rho(\widehat{\theta}, \widehat{p_{\mathrm{th}}})}{\partial \widehat{\theta}}\right\} \widetilde{\theta} \, \mathrm{d}v$$

$$+ \int_{\Omega} \left(-\frac{\widehat{p_{\mathrm{th}}}}{\widehat{\rho}\widehat{\theta}} + \lambda_2\right) \frac{\partial \rho(\widehat{\theta}, \widehat{p_{\mathrm{th}}})}{\partial \widehat{p_{\mathrm{th}}}} \widetilde{p_{\mathrm{th}}} \, \mathrm{d}v. \tag{79}$$

Since we want the derivative to vanish for arbitrary $\widetilde{p_{\mathrm{th}}}$, we see that we need to fix the second Lagrange multiplier λ_2 as

$$\lambda_2 = \frac{\widehat{p_{\mathrm{th}}}}{\widehat{\rho}\widehat{\theta}}. \tag{80}$$

With this choice of λ_2 we can revisit the first integral in (79), and we see that

$$\widehat{\rho}\left(\frac{\partial \eta(\widehat{\theta}, \widehat{p_{\mathrm{th}}})}{\partial \widehat{\theta}} - \lambda_1 \frac{\partial e(\widehat{\theta}, \widehat{p_{\mathrm{th}}})}{\partial \widehat{\theta}}\right) - \lambda_2 \frac{\partial \rho(\widehat{\theta}, \widehat{p_{\mathrm{th}}})}{\partial \widehat{\theta}}$$

$$= \widehat{\rho}\left(\frac{\partial \eta(\widehat{\theta}, \widehat{\rho})}{\partial \widehat{\theta}} - \lambda_1 \frac{\partial e(\widehat{\theta}, \widehat{\rho})}{\partial \widehat{\theta}}\right) + \widehat{\rho}\left(\frac{\partial \eta(\widehat{\theta}, \widehat{\rho})}{\partial \widehat{\rho}} - \lambda_1 \frac{\partial e(\widehat{\theta}, \widehat{\rho})}{\partial \widehat{\rho}}\right) \frac{\partial \rho(\widehat{\theta}, \widehat{p_{\mathrm{th}}})}{\partial \widehat{\theta}} - \lambda_2 \frac{\partial \rho(\widehat{\theta}, \widehat{p_{\mathrm{th}}})}{\partial \widehat{\theta}} = 0, \tag{81}$$

where we have used identities (71) and (77) and the formulae for the Lagrange multiplies.

Consequently, the Lyapunov type functional for nonlinear stability analysis of stationary spatially homogeneous steady state in a compressible Navier–Stokes–Fourier fluid is given by the formula

$$\mathcal{V}_{\mathrm{eq}} = -\int_{\Omega} \rho\eta \, \mathrm{d}v + \frac{1}{\widehat{\theta}} \int_{\Omega} \left(\frac{1}{2}\rho|\boldsymbol{v}|^2 + \rho e - \widehat{\rho}\widehat{e}\right) \mathrm{d}v + \frac{\widehat{p_{\mathrm{th}}}}{\widehat{\rho}\widehat{\theta}} \int_{\Omega} (\rho - \widehat{\rho}) \, \mathrm{d}v. \tag{82}$$

Note that from the perspective of generalisation to thermodynamically open systems, see [**P1**], it is convenient to use an equivalent functional $\mathcal{V}_{\mathrm{meq}}$ that is obtained from $\mathcal{V}_{\mathrm{eq}}$ by multiplication via the constant value $\widehat{\theta}$, that is

$$\mathcal{V}_{\mathrm{meq}} = -\int_{\Omega} \widehat{\theta}\rho\eta \, \mathrm{d}v + \int_{\Omega} \left(\frac{1}{2}\rho|\boldsymbol{v}|^2 + \rho e - \widehat{\rho}\widehat{e}\right) \mathrm{d}v + \int_{\Omega} \frac{\widehat{p_{\mathrm{th}}}}{\widehat{\rho}} (\rho - \widehat{\rho}) \, \mathrm{d}v. \tag{83}$$

(The term $\widehat{\rho}\widehat{e}$ can be replaced by $\rho\widehat{e}$ in virtue of the mass conservation constraint and the fact that $\widehat{e}$ is a constant.) In particular, if we consider the calorically perfect ideal gas with the Helmholtz free energy in the form

$$\psi(\theta, \rho) =_{\mathrm{def}} -c_{\mathrm{V,ref}}\theta\left(\ln\frac{\theta}{\widehat{\theta}} - 1\right) + c_{\mathrm{V,ref}}\theta(\gamma - 1)\ln\frac{\rho}{\widehat{\rho}} - c_{\mathrm{V,ref}}\widehat{\theta}, \tag{84}$$

where $c_{\mathrm{V,ref}}$ is the specific heat capacity at constant volume (a constant) and γ is the adiabatic exponent, then the functional (83) reduces to

$$\mathcal{V}_{\mathrm{meq}} = \int_{\Omega} \rho c_{\mathrm{V,ref}}\widehat{\theta}\left(\frac{\theta}{\widehat{\theta}} - 1 - \ln\frac{\theta}{\widehat{\theta}}\right) \mathrm{d}v + \int_{\Omega} \widehat{\rho}\widehat{\theta}(\gamma - 1)\left(\frac{\rho}{\widehat{\rho}}\ln\frac{\rho}{\widehat{\rho}} - \frac{\rho}{\widehat{\rho}} - 1\right) \mathrm{d}v. \tag{85}$$

It is straightforward to check that the functional is nonnegative, and that it vanishes if and only if $\rho = \widehat{\rho}$ and $\theta = \widehat{\theta}$. See also Dostalík and Průša [2022] for further comments regarding leading order approximation of the functional and the relation of the leading order approximation to the standard *linearised* stability theory (infinitesimal perturbations).

2.1.4. *Example.* A relatively involved application of the procedure for construction of Lyapunov type functionals outlined is Section 2.1.2 is given in our work Dostalík et al. [2020], where we investigate the classical micro-macro model for compressible dilute polymeric fluids (53), see, for example, [Öttinger and Grmela, 1997, Section III], and wherein the equation of state for the solvent is taken from Le Métayer and Saurel [2016].

In this case the state space consists of the solvent density ρ_s, velocity $\boldsymbol{v}$, temperature θ_s and the configurational distribution function φ. If we decompose the state variables to the spatially homogeneous stationary part $\widehat{\boldsymbol{W}} =_{\mathrm{def}} \left[\widehat{\boldsymbol{v}}, \widehat{\rho_\mathrm{s}}, \widehat{\theta_\mathrm{s}}, \widehat{\varphi}\right]$ and the perturbation $\widetilde{\boldsymbol{W}} =_{\mathrm{def}} \left[\widetilde{\boldsymbol{v}}, \widetilde{\rho_\mathrm{s}}, \widetilde{\theta_\mathrm{s}}, \widetilde{\varphi}\right]$, that is

$$[\boldsymbol{v}, \rho_\mathrm{s}, \theta_\mathrm{s}, \varphi] = \left[\widehat{\boldsymbol{v}}, \widehat{\rho_\mathrm{s}}, \widehat{\theta_\mathrm{s}}, \widehat{\varphi}\right] + \left[\widetilde{\boldsymbol{v}}, \widetilde{\rho_\mathrm{s}}, \widetilde{\theta_\mathrm{s}}, \widetilde{\varphi}\right], \tag{86}$$

then the functional constructed by the method outlined above reads

$$
\begin{aligned}
\mathcal{V}_{\mathrm{meq}}\left(\widetilde{\rho_\mathrm{s}}, \widetilde{\theta_\mathrm{s}}, \widetilde{\varphi}, \widetilde{\boldsymbol{v}} \,\middle\|\, \widehat{\rho_\mathrm{s}}, \widehat{\theta_\mathrm{s}}, \widehat{\varphi}, \widehat{\boldsymbol{v}}\right) =_{\mathrm{def}} &\int_\Omega \frac{1}{2}\rho_\mathrm{s}\left|\boldsymbol{v}\right|^2 \mathrm{d}v \\
+ \int_\Omega \rho_\mathrm{s} c_{\mathrm{V,s}}\widehat{\theta_\mathrm{s}}\left[\frac{\theta_\mathrm{s}}{\widehat{\theta_\mathrm{s}}} - 1 - \ln\left(\frac{\theta_\mathrm{s}}{\widehat{\theta_\mathrm{s}}}\right)\right]\mathrm{d}v &+ \int_\Omega c_{\mathrm{V,s}}(\gamma - 1)\widehat{\theta_\mathrm{s}}\left[\rho_\mathrm{s}\ln\left(\frac{\rho_\mathrm{s}}{\widehat{\rho_\mathrm{s}}}\frac{1 - b\widehat{\rho_\mathrm{s}}}{1 - b\rho_\mathrm{s}}\right) - \frac{\rho_\mathrm{s} - \widehat{\rho_\mathrm{s}}}{1 - b\widehat{\rho_\mathrm{s}}}\right]\mathrm{d}v \\
+ k_\mathrm{B}\widehat{\theta_\mathrm{s}}\int_\Omega &\left(\int_D M_{n_\mathrm{p}, \widehat{\theta_\mathrm{s}}}\left[\frac{\varphi}{M_{n_\mathrm{p}, \widehat{\theta_\mathrm{s}}}}\ln\left(\frac{\varphi}{M_{n_\mathrm{p}, \widehat{\theta_\mathrm{s}}}}\right) - \frac{\varphi}{M_{n_\mathrm{p}, \widehat{\theta_\mathrm{s}}}} + 1\right]\mathrm{d}\boldsymbol{q}\right)\mathrm{d}v \\
&+ k_\mathrm{B}\widehat{\theta_\mathrm{s}}\int_\Omega \widehat{n_\mathrm{p}}\left[\frac{n_\mathrm{p}}{\widehat{n_\mathrm{p}}}\ln\left(\frac{n_\mathrm{p}}{\widehat{n_\mathrm{p}}}\right) - \frac{n_\mathrm{p}}{\widehat{n_\mathrm{p}}} + 1\right]\mathrm{d}v, \quad (87)
\end{aligned}
$$

where $n_\mathrm{p}(t, \boldsymbol{x}) =_{\mathrm{def}} \int_D \varphi(t, \boldsymbol{x}, \boldsymbol{q})\,\mathrm{d}\boldsymbol{q}$ denotes the polymer number density again decomposed to the spatially homogeneous stationary part and the perturbation $n_\mathrm{p} = \widehat{n_\mathrm{p}} + \widetilde{n_\mathrm{p}}$, and where

$$M_{n_\mathrm{p}, \theta_\mathrm{s}} =_{\mathrm{def}} n_\mathrm{p}\frac{\mathrm{e}^{-\frac{U\left(\frac{1}{2}\left|\frac{\boldsymbol{q}}{q_{\mathrm{ref}}}\right|^2\right)}{k_\mathrm{B}\theta_\mathrm{s}}}}{\int_D \mathrm{e}^{-\frac{U\left(\frac{1}{2}\left|\frac{\boldsymbol{q}}{q_{\mathrm{ref}}}\right|^2\right)}{k_\mathrm{B}\theta_\mathrm{s}}}\,\mathrm{d}\boldsymbol{q}} \tag{88}$$

denotes the Maxwellian for the given solvent temperature θ_s and polymer number density n_p; for thorough discussion see Dostalík et al. [2020]. Furthermore, if we ignore quantities φ and n_p, that is the last two terms on the right-hand side, we get the functional for the solvent only, which is a functional for the compressible Navier–Stokes–Fourier fluid with the corresponding equation of state.

2.2. Thermodynamically open systems.

2.2.1. *Expected qualitative behaviour.* More interesting class of thermodynamical systems is the class of open systems. The open systems that can exchange energy/mass with the outside environment, see Figure 5 for a sketch of such a system, and, typically, the dynamics of these systems is externally forced via the interaction with outside environment.

Since these systems are forced, one can typically observe a non-trivial steady state in these systems. (Non-trivial flow structure, non-trivial temperature distribution—Rayleigh–Bénard convection or Taylor–Couette flow are good examples of such systems.) Regarding the perturbations to the given steady state and their long-time behaviour, two scenarios are possible, see Figure 5. Either the perturbations vanish as the time goes to infinity, and the steady state is recovered, or the perturbations grow in time, and they destroy the original steady state and a new structure emerges. Usually, the long-time behaviour of the perturbations depends on the strength of the external forcing that is characterised using some dimensionless parameters such as the Rayleigh number, the Reynolds number or the Weissenberg number.
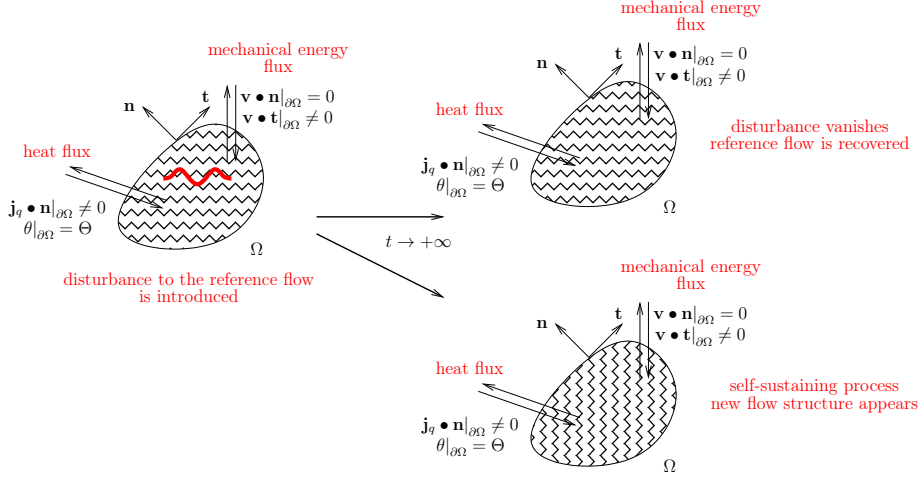
FIGURE 5. Thermodynamically open system.

2.2.2. *Lyapunov type functional.* The stability analysis of steady states in thermodynamically open systems can be—from the mathematical point of view—again based on the construction of a suitable Lyapunov functional. However, the functional must be constructed differently than in the case of thermodynamically isolated systems. The insufficiency of the construction that worked for *isolated systems* is obvious, because

(1) The steady state in an open system is typically spatially inhomogeneous, which means that, for example, the steady temperature field $\widehat{\theta}$ can be a *function of position.* Consequently, formulae of type (62) with Lagrange multipliers (73) and (80) do not define functionals.

(2) Open systems are interacting with outside environment, and hence there are nontrivial fluxes through the system boundary. In particular the entropy flux through the boundary can be nontrivial, and the net entropy growth (67) can not be guaranteed at all time instants.

The construction of a functional suitable for monitoring the progress towards the target steady state can be addressed by the *affine correction* of the functional used in the case of thermodynamically isolated system. This is a technique used in the theory of hyperbolic systems, see Ericksen [1966], Dafermos [1979], Serre and Vasseur [2016] and comments in [**P1**]. (Note however that in the theory of hyperbolic systems the stability usually means continuous dependence on initial state and supply terms, *not* the asymptotic stability.) The construction goes as follows. If we have a functional $\mathcal{V}_{\mathrm{meq}}$ suitable for the stability analysis of the spatially homogeneous stationary state in an *isolated* system, we construct the functional $\mathcal{V}_{\mathrm{neq}}$ that can serve for stability analysis of the steady state in the corresponding *open* system via the formula

$$\mathcal{V}_{\mathrm{neq}}\big(\widetilde{\boldsymbol{W}}_{\mathrm{neq}}\big\|\,\widehat{\boldsymbol{W}}_{\mathrm{neq}}\big) =_{\mathrm{def}} \mathcal{V}_{\mathrm{meq}}\big(\widehat{\boldsymbol{W}}_{\mathrm{neq}} + \widetilde{\boldsymbol{W}}_{\mathrm{neq}}\big) - \mathcal{V}_{\mathrm{meq}}\big(\widehat{\boldsymbol{W}}_{\mathrm{neq}}\big) - \mathrm{D}_{\boldsymbol{W}}\mathcal{V}_{\mathrm{meq}}(\boldsymbol{W})\big|_{\boldsymbol{W}=\widehat{\boldsymbol{W}}_{\mathrm{neq}}}\big[\widetilde{\boldsymbol{W}}_{\mathrm{neq}}\big], \quad (89)$$

where the symbol $\mathrm{D}_{\boldsymbol{W}}\mathcal{V}_{\mathrm{meq}}(\boldsymbol{W})\big|_{\boldsymbol{W}=\widehat{\boldsymbol{W}}_{\mathrm{neq}}}\big[\widetilde{\boldsymbol{W}}_{\mathrm{neq}}\big]$ again denotes the Gâteaux derivative of $\mathcal{V}_{\mathrm{meq}}$ at point $\widehat{\boldsymbol{W}}_{\mathrm{neq}}$ in the direction $\widetilde{\boldsymbol{W}}_{\mathrm{neq}}$, and where $\boldsymbol{W} = \widehat{\boldsymbol{W}}_{\mathrm{neq}} + \widetilde{\boldsymbol{W}}_{\mathrm{neq}}$ denotes the state variables decomposed to the steady state $\widehat{\boldsymbol{W}}_{\mathrm{neq}}$ and the perturbation $\widetilde{\boldsymbol{W}}_{\mathrm{neq}}$ with respect to the steady state.

Having identified a candidate for the monitoring of the evolution of the perturbation, we need to find the time derivative $\frac{\mathrm{d}\mathcal{V}_{\mathrm{neq}}}{\mathrm{d}t}$ of the proposed functional (89). However, *the time derivative apparently forces us to work with non-vanishing surface integrals.*

Indeed, we in principle need to evaluate the terms of the type $\frac{\mathrm{d}S}{\mathrm{d}t}$, which can, unlike in the case of thermodynamically isolated systems (67), contain the surface integral

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \int_{\Omega} \xi \,\mathrm{dv} - \int_{\partial\Omega} \boldsymbol{j}_{\eta} \bullet \boldsymbol{n} \,\mathrm{ds} = \int_{\Omega} \xi \,\mathrm{dv} + \int_{\partial\Omega} \kappa \frac{\nabla\theta}{\theta} \bullet \boldsymbol{n} \,\mathrm{ds}, \quad (90)$$

where we have used the standard formula for the entropy flux $\boldsymbol{j}_\eta = \frac{\boldsymbol{j}_q}{\theta} = -\kappa \frac{\nabla \theta}{\theta}$. If we were using the zero heat flux boundary condition,

$$\kappa \nabla \theta \bullet \boldsymbol{n}|_{\partial \Omega} = 0, \tag{91}$$

that is if we were dealing a with a thermally isolated system, the surface integral would vanish. But if deal with an thermally *open system*, that is if we for example prescribe the boundary condition for the temperature

$$\theta|_{\partial \Omega} = \theta_{\mathrm{bdr}}, \tag{92}$$

where θ_{bdr} is a given boundary temperature, then the product $\kappa \frac{\nabla \theta}{\theta} \bullet \boldsymbol{n}$ does not necessarily vanish. More importantly, the product has no definite sign, and its sign can dynamically change during the evolution of the system. Consequently, the "entropy growth" is lost, and it seems that time derivatives of the net quantities lead to the presence of surface integrals that are beyond our control.

Fortunately, functionals of type (89) include terms $\rho \widehat{\theta} \eta(\boldsymbol{W}) - \rho e(\boldsymbol{W})$, where $\widehat{\theta}$ denotes the (possibly spatially inhomogeneous) temperature at the target steady state. (The factor $\widehat{\theta}$ originates form the Lagrange multiplier in (82), see [**P1**] for details.) The time derivative of $\rho \widehat{\theta} \eta(\boldsymbol{W}) - \rho e(\boldsymbol{W})$ then typically involves the difference between the heat flux $\boldsymbol{j}_q$ and the entropy flux $\boldsymbol{j}_\eta$. If both fluxes are related through the classical formula $\boldsymbol{j}_\eta = \frac{\boldsymbol{j}_q}{\theta}$, then it holds

$$\widehat{\theta} \operatorname{div} \boldsymbol{j}_\eta - \operatorname{div} \boldsymbol{j}_q = \widehat{\theta} \operatorname{div} \left(\frac{\boldsymbol{j}_q}{\widehat{\theta} + \widetilde{\theta}} \right) - \operatorname{div} \boldsymbol{j}_q = \operatorname{div} \left(\left[\frac{\widehat{\theta}}{\widehat{\theta} + \widetilde{\theta}} - 1 \right] \boldsymbol{j}_q \right) - \nabla \widehat{\theta} \bullet \frac{\boldsymbol{j}_q}{\widehat{\theta} + \widetilde{\theta}}. \tag{93}$$

Since (92) implies that the temperature perturbation $\widetilde{\theta}$ vanishes on the boundary, we see that the first term on the right-hand side of (93) vanishes upon integration over the vessel Ω by virtue of the Stokes theorem. On the other hand, the second term on the right-hand side does not in general vanish. (It might vanish for example in the case of a system immersed in a *thermal bath* wherein θ_{bdr} is a constant in space.) Nonetheless, the second term on the right-hand side of (93) leads to a *volumetric term* in the formula for the time derivative of the functional, which makes the time derivative of the functional tractable.

2.2.3. *Examples.* Particular examples of functionals constructed using the procedure outlined in Section 2.2.2 is the functional

$$\mathcal{V}_{\mathrm{neq}} \left(\widetilde{\boldsymbol{W}} \,\|\, \widehat{\boldsymbol{W}} \right) = \int_\Omega \left[\rho c_{\mathrm{V,ref}} \widehat{\theta} \left[\frac{\widetilde{\theta}}{\widehat{\theta}} - \ln \left(1 + \frac{\widetilde{\theta}}{\widehat{\theta}} \right) \right] + \frac{1}{2} \rho \,|\widetilde{\boldsymbol{v}}|^2 \right] \mathrm{dv}, \tag{94}$$

which is the functional used in [**P2**] in stability analysis of motion of incompressible Navier–Stokes–Fourier fluid in a vessel with walls kept at spatially nonuniform temperature, and the family of functionals used in [**P3**] in the same setting but for a class of viscoelastic rate-type fluids.

The problem considered in [**P2**] and in [**P3**] is apparently very simple. A fluid—either an incompressible Navier–Stokes–Fourier fluid or an incompressible viscoelastic rate-type fluid—is occupying a mechanically isolated vessel with walls kept at *spatially non-uniform temperature*, see Figure 6c for a sketch. Based upon everyday experience, the fluid is in the long run expected to reach the spatially inhomogeneous steady state. Irrespective of the initial conditions the velocity field is expected to vanish, and the temperature field is expected to reach the steady state given by the solution of the steady heat equation.

Interestingly, this simple observation is difficult to prove using the corresponding governing equations. For example, the popular *energy method* for nonlinear stability analysis, see Straughan [2004], fails in this setting. The main difficulties are the presence of the dissipative heating term in the evolution equation for temperature, and, as we have already noted, the lack of control on the heat fluxes through the boundary. The proof presented in [**P2**] and in [**P3**] basically follows the approach outlined above, but it adds one important ingredient. The proof exploits the fact that *the stability result must not depend on the choice of temperature scale*. The ambiguity in the choice of temperature scale then allows one to construct a whole family of Lyapunov type functionals that can be combined together in order to overcome some quantitative issues.

Furthermore, the analysis in [**P2**] reveals that if the wall temperature is spatially homogeneous, that is if the vessel is immersed in a thermal bath, see Figure 6b, then all the technical difficulties are essentially gone. In this case the spatially homogeneous boundary condition admits a spatially homogeneous steady state $\widehat{\theta}$, and if $\nabla \widehat{\theta} = 0$, then all the difficult-to-handle terms vanish and the
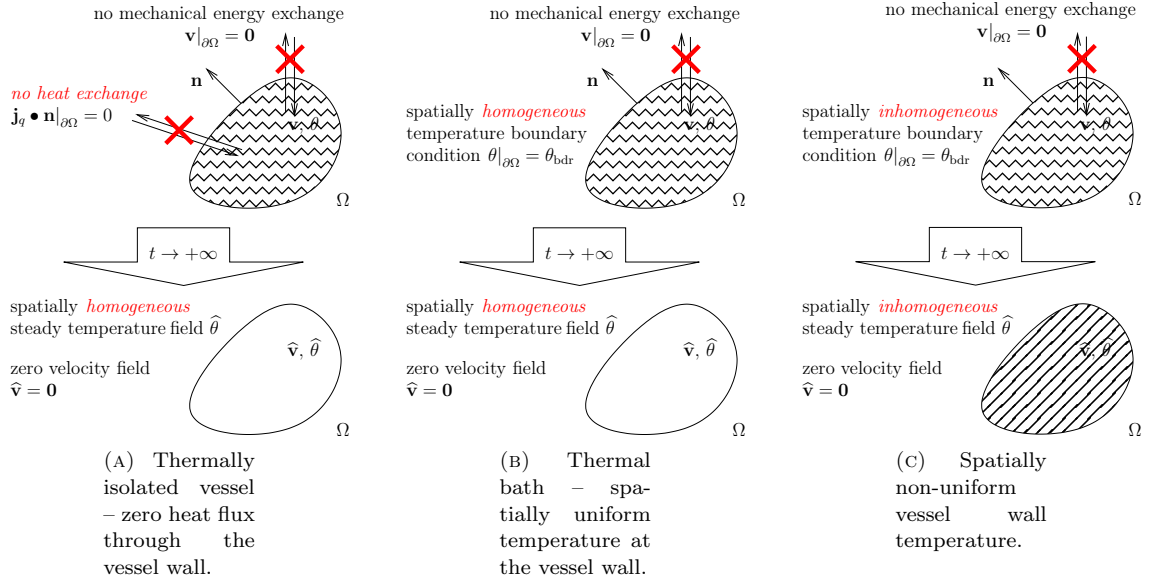
FIGURE 6. Long time behaviour under various types of temperature boundary conditions.

proof greatly simplifies. The same holds for thermally isolated system, see Figure 6a. This observation again documents that the *boundary conditions* are as important as the governing equations themselves. Depending on the choice of boundary conditions, the difficulty of stability analysis of the given system can change considerably.

In [**P4**] we consider a purely mechanical problem of stability of flow of Giesekus viscoelastic rate-type fluid. (The Giesekus model is a variant of Oldroyd-B model with a slightly stronger dissipation.) The governing equations for mechanical variables read

$$\operatorname{div} \boldsymbol{v} = 0, \tag{95a}$$

$$\rho \frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = \operatorname{div} \mathbb{T}, \tag{95b}$$

$$\nu_1 \overline{\mathbb{B}_{\kappa_{p(t)}}^{\triangledown}} = -\mu \left[\alpha \mathbb{B}_{\kappa_{p(t)}}^2 + (1 - 2\alpha) \mathbb{B}_{\kappa_{p(t)}} - (1 - \alpha) \mathbb{I} \right], \tag{95c}$$

and the Cauchy stress tensor is given by the familiar formulae

$$\mathbb{T} =_{\mathrm{def}} -p\mathbb{I} + \mathbb{T}_\delta, \tag{95d}$$

$$\mathbb{T}_\delta =_{\mathrm{def}} 2\nu \mathbb{D} + \mu \left(\mathbb{B}_{\kappa_{p(t)}} \right)_\delta. \tag{95e}$$

The symbol α denotes a material parameter, and we consider $\alpha \in (0, 1)$. For $\alpha = 0$ the model reduces to the Oldroyd-B model, but this case is not covered in the stability analysis.

The fluid is externally driven by an influx of mechanical energy, in particular we consider flows driven by moving boundaries. This corresponds, for example, to the classical setting of flow in between two rotating concentric cylinders (Taylor–Couette flow). The governing equations are assumed to have a steady solution with a steady velocity field $\widehat{\boldsymbol{v}}$ and a steady $\widehat{\mathbb{B}_{\kappa_{p(t)}}}$ field. The task is to investigate the nonlinear stability of such solution.

In this case the functional constructed by the method outlined above reads

$$\mathcal{V}_{\mathrm{neq}} \left(\widetilde{\boldsymbol{W}} \, \| \, \widehat{\boldsymbol{W}} \right) = \int_\Omega \frac{1}{2} \rho \, |\widetilde{\boldsymbol{v}}|^2 \, \mathrm{dv} + \int_\Omega \frac{\mu}{2} \left[-\ln \det \left(\mathbb{I} + \widehat{\mathbb{B}_{\kappa_{p(t)}}}^{-1} \widetilde{\mathbb{B}_{\kappa_{p(t)}}} \right) + \operatorname{Tr} \left(\widehat{\mathbb{B}_{\kappa_{p(t)}}}^{-1} \widetilde{\mathbb{B}_{\kappa_{p(t)}}} \right) \right] \mathrm{dv}. \tag{96}$$

We note that the functional is again *not quadratic* in perturbation $\widetilde{\mathbb{B}_{\kappa_{p(t)}}}$. In [**P4**] we show that the time derivative of the functional is estimated from above as

$$\frac{\mathrm{d}\mathcal{V}_{\mathrm{neq}}}{\mathrm{d}t}\left(\widetilde{\boldsymbol{W}}\,\middle\|\,\widehat{\boldsymbol{W}}\right) \le C_1 \|\nabla\widetilde{\boldsymbol{v}}\|^2_{L^2(\Omega)} + C_2\left\|\widetilde{\mathbb{B}_{\kappa_{p(t)}}}\right\|^2_{L^2(\Omega)}, \tag{97}$$

where we denote

$$C_1 =_{\mathrm{def}} -\frac{1}{\mathrm{Re}} + C_P \sup_{\boldsymbol{x}\in\Omega}\left|\lambda_{\min}(\widehat{\mathbb{D}})\right| + \frac{\Xi}{2}\sup_{\boldsymbol{x}\in\Omega}\left|\widehat{\mathbb{B}_{\kappa_{p(t)}}}^{-1} - \mathbb{I}\right| + C_P\frac{\Xi}{4}\sup_{\boldsymbol{x}\in\Omega}\left|\widehat{\mathbb{B}_{\kappa_{p(t)}}}^{-1}\right|^2\sup_{\boldsymbol{x}\in\Omega}\left|\nabla\widehat{\mathbb{B}_{\kappa_{p(t)}}}\right|, \tag{98a}$$

$$C_2 =_{\mathrm{def}} -\alpha\frac{\Xi}{2\mathrm{Wi}}\inf_{\boldsymbol{x}\in\Omega}\lambda_{\min}(\widehat{\mathbb{B}_{\kappa_{p(t)}}}^{-1}) + \frac{\Xi}{2}\sup_{\boldsymbol{x}\in\Omega}\left|\widehat{\mathbb{B}_{\kappa_{p(t)}}}^{-1} - \mathbb{I}\right| + \frac{\Xi}{4}\sup_{\boldsymbol{x}\in\Omega}\left|\widehat{\mathbb{B}_{\kappa_{p(t)}}}^{-1}\right|^2\sup_{\boldsymbol{x}\in\Omega}\left|\nabla\widehat{\mathbb{B}_{\kappa_{p(t)}}}\right|, \tag{98b}$$

and where $\lambda_{\min}(\cdot)$ denotes the minimal eigenvalue of the corresponding matrix and C_P denotes the domain dependent constant from Friedrichs–Poincaré inequality. The estimate holds unconditionally, that is irrespective of the initial size of the perturbation. Clearly, if the Weissenberg number Wi and the Reynolds number Re in (98) are *small* enough, the constants C_1 and C_2 are negative and the steady flow is stable *with respect to any perturbation*.

On the other hand, when one of the constants is positive one can *conjecture* that the flow is, at least for some perturbations, unstable. Interestingly, this observation is in line with the phenomenon of *elastic turbulence*, see, for example, Groisman and Steinberg [2000]. The *elastic turbulence* is a phenomenon where one can observe "turbulent flow" at extremely small Reynolds numbers. This means that the turbulent behaviour is not due to the standard convective nonlinearity in the balance of linear momentum whose strength is measured by the Reynolds number. The turbulent behaviour is due to the *elastic component* of the fluid, which is measured by the *Weissenberg number*. Our results is, however, in an opposite direction. We are able to identify the safe values—no instability— of Weissenberg number and Reynolds number. For such values we know that the instability can not be triggered and the transition to a turbulent state can not happen. What happens behind this range of safe values is a question for further research.

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