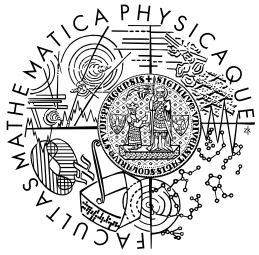


FACULTY
OF MATHEMATICS
AND PHYSICS
Charles University

**MASTER THESIS**

Bc. Vojtěch Miloš

# Modelling of viscoelastic materials with temperature dependence

Mathematical Institute, Charles University

| | |
|---|---|
| Supervisor of the master thesis: | RNDr. Jaroslav Hron, Ph.D. |
| Study programme: | Mathematics |
| Study branch: | Mathematical Modelling in Physics and Technology |

Prague 2016

I am very thankful to my supervisor Jaroslav Hron and consultant Ondřej Souček for their guidance, insight and all the helpful remarks and comments. I would also like to thank my family for their great support.

I declare that I carried out this master thesis independently, and only with the cited sources, literature and other professional sources.

I understand that my work relates to the rights and obligations under the Act No. 121/2000 Coll., the Copyright Act, as amended, in particular the fact that the Charles University in Prague has the right to conclude a license agreement on the use of this work as a school work pursuant to Section 60 paragraph 1 of the Copyright Act.

In ..... date .....  signature of the author

Název práce: Modelování viskoelastických materialů s teplotní závislostí

Autor: Bc. Vojtěch Miloš

Katedra: Matematický Ústav UK

Vedoucí diplomové práce: RNDr. Jaroslav Hron, Ph.D., Katedra numerické matematiky

Abstrakt: Materiály jako sklo, asfalt, polymery nebo zemská kůra vykazují chování, které nelze popsat modelem pro viskózní tekutinu ani modelem pro pevnou látku. Existují modely, které jsou schopny tyto tzv. viskoelastické jevy zachytit mnohem lépe, nicméně tyto modely většinou předpokládají konstantní teplotu. V mnoha případech, například ve sklářství nebo v geofyzice, vlastnosti viskoelastického materiálu silně závisí na teplotě a právě tyto změny je třeba popsat. V praxi se používají viskoelastické modely, které uvažují závislost materiálových parametrů na teplotě, nicméně při popisu evoluce teploty nezohledňují viskoelastickou povahu materiálu. Cílem této práce je odvození termodynamicky konzistentních viskoelastických modelů s materiálovými parametry závislými na teplotě a příslušnou evoluční rovnicí pro teplotu, implementace těchto modelů a provedení jednoduchých testových simulací.

Klíčová slova: viskoelasticita, teplotní závislost

Title: Modelling of viscoelastic materials with temperature dependence

Author: Bc. Vojtěch Miloš

Department: Mathematical Institute, Charles University

Supervisor: RNDr. Jaroslav Hron, Ph.D., Department of Numerical Mathematics

Abstract: Materials such as asphalt, polymers or the Earth's crust tend to behave in a way that can be described neither with a model of viscous fluid, nor a model from solid mechanics. There are indeed models capable of capturing these so called viscoelastic phenomena far better, but they are based on the presumption of constant temperature. In many cases, e.g. in the glass industry or in geophysics, the properties of a viscoelastic material strongly depend on temperature. That is why it is precisely these changes that need to be described. There are viscoelastic models used in practice that take into account the material parameters' dependence on temperature, however, they do not consider the viscoelastic nature of the material when describing the temperature evolution. The objective of this thesis is to derive thermodynamically consistent viscoelastic models with temperature dependent parameters and the appropriate evolution equation for temperature, implementation of the models and computing simple test simulations.

Keywords: viscoelasticity, temperature dependence

# Contents

# Introduction

Only an experienced glassmaker knows how to cool down a big piece of glass quickly and efficiently without cracking it. During the cooling process, there are very complicated quality changes which are very hard to capture by a physical or mathematical model. Glass changes its consistency from melted viscous fluid to elastic solid but the question is how to describe the state of matter in the middle of this process.

The material property which exhibits both viscous and elastic behaviour is called viscoelasticity. There are widely used models, for example the Oldroyd model, that describe the viscoelastic response of a material undergoing deformation but they do so under the assumption that the temperature is constant. This isothermal approximation is sufficient in many applications. Yet, there also are cases in which the influence of temperature is fundamental, for example in glass industry or in polymer science. The few existing viscoelastic models with temperature dependent material constants that are able to capture experiment data, for example [6], were developed without paying much attention to the evolution of temperature reflecting the viscoelastic character of the material, and some models do not pay attention to the thermodynamic consistency of the model at all. In this thesis, we show how to derive a thermodynamic consistent viscoelastic model with general temperature dependent coefficients and the evolution equation for temperature resulting from the nature of the viscoelastic model. For this purpose, we use the thermodynamic framework proposed by Rajagopal and Srinivasa (see [12]) that is based on the notion of natural configuration and the principle of maximal rate of entropy production, and we extend it with temperature dependent coefficients and derive an appropriate equation for temperature evolution. At the beginning, we define two scalar functions - the rate of dissipation $\Xi$ and the thermodynamic potential, e. g. free energy $\psi$ -, insert them in the framework and obtain constitutive relations for the Cauchy stress tensor $T$ and the heat flux $q$, which encloses the system of governing equations.

This framework was used in the doctoral thesis of Karel Tůma [15] with the assumption that the temperature is constant. He derived the Oldoroy-B model and also the nonlinear model Quad1 in order to capture data from a torque experiment with asphalt binder. We follow up his work by deriving a temperature dependent models, T-Oldroyd (thus also T-Maxwell) and T-Quad1, to show that a generalization of the framework is possible.

Originally, the idea to explore this topic arose from Karel Tůma's doctoral thesis and also from a cooperation with a glassmaking company. They suggested to perform oscillatory tests on a rectangular piece of glass in order to be able to choose (or develop) an appropriate model and fit the parameters. The method of determining characteristics of the material undergoing sinusoidal deformation is called Dynamic mechanical analysis (DMA) and it uses oscillatory material (complex) constants $G^*(\omega)$ and $J^*(\omega)$. Hence, in the first chapter, we give an overview of the basic viscoelastic models including the plots of their oscillatory constants. The very experiment was - in the end - not carried out but we still include the overview since it can be useful for further research. The rest of the

first chapter focuses on the 1D mechanical analogues of viscoelasticity - a linear spring and a dashpot (or damper) - with the influence of temperature. We look at the system of springs and dashpots from the thermodynamic point of view, define its free energy and derive the evolution equation for temperature. Since we use a very similar approach in the case of real models, the one for mechanical analogues can serve as an exemplary derivation. The derived models are tested in oscillatory experiments and can provide an intuitive insight in the behaviour of thermal viscoelasticity.

The proper derivation for a real fluid (or continuum in general) is done in the second chapter. It starts from the balance equations and continues with the derivation of a temperature evolution equation. Using the notion of natural configuration, we split the deformation on elastic end dissipative part. After supposing the response of the material to be neo-Hookean (both cases, incompressible and compressible) and defining two different rates of dissipation, we use the principle of maximal rate of entropy production and obtain three incompressible models mentioned above, T-Oldroyd, T-Maxwell and T-Quad1.

Our goal is also performing numerical simulations with derived models. In order to do so, the third chapter starts with the weak formulation of T-Oldroyd and T-Quad1 models. Then we describe the implementation of Finite element method and is followed by standard benchmark for verification of the code written in the with aid of the project FEniCS. If we want to simulate deforming objects, which can be for example oscillating piece of material, and run the simulation on a static computational mesh, we can use the Lagrange description instead of Eulerian. However, in the case of larger deformation, more robust approach should be considered hence we use Arbitrary Lagrangian-Eulerian (ALE) method.

# 1. 1D Viscoelastic Toys

In this chapter, we study viscoelastic mechanical analogues undergoing oscillatory deformations and present an overview of basic models together with plots of the quantities connected with their oscillatory material constants. The second section, the system of springs and dashpots is equipped by thermodynamic quantities in order to get some interesting behaviour for example in oscillatory tests.

## 1.1 Spring and Dashpot

Linear viscoelastic models have their origin in mechanical analogues. These are defined by the relation between the pulling stress $\sigma$ and relative elongation or strain $\epsilon$. Linear spring is characterized by the relation

$$\sigma = k\epsilon,$$

where $k$ is stiffness of the spring. Linear dashpot is defined by the relation

$$\sigma = \nu\dot{\epsilon},$$

where $\nu$ is viscosity of the dashpot and $\dot{\epsilon}$ denotes time derivative of $\epsilon$. One can link springs and dashpot in parallel or in series to obtain different viscoelastic models. The famous ones are Maxwell model and Kelvin-Voigt model which consist of one spring and one dashpot in series and parallel, respectively. Besides, in this chapter we are interested in Oldroyd and Burgers models.

There are two basic tests revealing and describing the behaviour of viscoelastic models and materials.

**Creep test** is based on applying a step stress $\sigma_0$ in a specimen at time $t = 0$ and observing the elongation $\epsilon(t)$ of the specimen in time.

**Stress relaxation test** is based on subjecting a specimen to step strain $\epsilon_0$ and observing corresponding stress relaxation curve $\sigma(t)$.

An overview of these tests for the basic models are properly done for example in the book [16] or in doctoral thesis [15] together with description of other viscoelastic effects, hence we do not present it here. However, we are interested in small amplitude oscillation tests due to the growing importance of Dynamic mechanical analysis (DMA)(also known as Dynamic mechanical spectroscopy). DMA is a method to characterize a material properties. It is based on applying a sinusoidal strain

$$\epsilon(t) = \epsilon_0 \sin(\omega t)$$

on a specimen and observing the stress response in the form

$$\sigma(t) = \sigma_0 \sin(\omega t + \delta).$$

The amplitude of oscillation $\epsilon_0$ is small enough that the material response can be considered to be in the linear range. The specimen undergoes oscillatory deformation for many different frequencies $\omega$ (and possibly at different temperatures $\theta$) and one can determine the complex modulus $G^*(\omega, \theta)$. Let us remark, that one can do it in an opposite way and after applying sinusoidal stress $\sigma(t)$ can observe the response in strain $\epsilon(t)$. In this case one obtains other material coefficient complex compliance $J^*(\omega, \theta)$. A definition of complex modulus and compliance as well as their properties can be found in the following. For more details about DMA, see [11].

### 1.1.1 Small Amplitude Oscillation

In this section we introduce a material response functions complex modulus $G^*(\omega)$ and complex compliance $J^*(\omega)$ widely used in experiments based on small amplitude oscillations and their explicit form for several models. Here, we are dealing with an isotermal case. More details about this topic such as a proper derivation of all terms used here can be found in the book [16].

#### Relaxation function and creep compliance

Assume we have a one-dimensional linear viscoelastic model defined by a constitutive equation [1] - the relation between $\sigma$ and $\epsilon$, stress and strain respectively. Let us denote Heaviside step function as $H_1(t)$ with $H_1(0) = 1$. If we then assume a standard step strain

$$\hat{\epsilon}(t) := \epsilon_0 H_1(t)$$

and $\hat{\sigma}(t)$ is an appropriate stress response given by the considered constitutive equation, an important function - relaxation function $G(t)$ is defined by

$$G(t) := \frac{\hat{\sigma}(t)}{\epsilon_0}.$$

It can be shown that a response to an arbitrary strain history $\epsilon(t)$ for $t \geq 0$ can be expressed by this 'canonical' response $G(t)$ as

$$\sigma(t) = G(t)\epsilon(0) + \int_0^t G(t-s)\dot{\epsilon}(s)ds.$$

Similarly, if we assume step stress

$$\hat{\sigma}(t) := \sigma_0 H_1(t),$$

the creep compliance $J(t)$ is defined by

$$J(t) := \frac{\hat{\epsilon}(t)}{\sigma_0},$$

[1] For example

$$\frac{\dot{\sigma}(t)}{k} + \frac{\sigma(t)}{\nu} = \dot{\epsilon}(t)$$

with viscosity $\nu$ and stiffness $k$ is the constitutive equation for the Maxwell model.

where $\hat{\epsilon}(t)$ is appropriate strain response. In the same manner, a strain response to an arbitrary stress history $\sigma(t)$ for $t \geq 0$ can be expressed as

$$\epsilon(t) = J(t)\sigma(0) + \int_0^t J(t-s)\dot{\sigma}(s)ds.$$

It can be shown that $G(t)$ and $J(t)$ are coupled by the relation

$$1 = G(t)J(0) + \int_0^t G(t-s)\dot{J}(s)ds.$$

**Complex modulus**

Let us consider a material subjected to oscillatory strain history

$$\epsilon_s(t) = \epsilon_0 \sin(\omega t) \quad \text{or} \quad \epsilon_c(t) = \epsilon_0 \cos(\omega t).$$

Both strain histories can be regarded as the imaginary and real parts of the complex strain history

$$\epsilon(t) = \epsilon_0 e^{i\omega t} = \epsilon_0(\cos(\omega t) + i\sin(\omega t),$$

where $\epsilon_0$ is the amplitude and $\omega$ is the frequency. If we expect the appropriate sinusoidal stress response in the form

$$\sigma(t) := \sigma_c(t) + i\sigma_s(t),$$

it can be shown that there exist a function - complex modulus $G^*(\omega)$ such as

$$\sigma(t) = G^*(\omega)\epsilon(t).$$

Note that the appropriate stress response develops into sinusoidal shape for sufficiently large time $t$. When performing an experiment it is necessary to wait until the shape of stress response becomes sinusoidal.

Let us note several facts about complex modulus.

- Complex modulus can be written in algebraic form as

  $$G^*(\omega) = G'(\omega) + iG''(\omega),$$

  where $G'(\omega)$ and $G''(\omega)$ are called storage modulus and loss modulus respectively. Alternatively it can be expressed in polar form

  $$G^*(\omega) = |G^*(\omega)|e^{i\delta(\omega)},$$

  where $\delta(\omega) = \text{arctg}(G''(\omega)/G'(\omega))$ performs a phase difference between sinuses $\sigma(t)$ and $\epsilon(t)$ and $|G^*(\omega)| = \sqrt{G'(\omega)^2 + G''(\omega)^2}$ describes the ratio of their amplitudes. One can then write

  $$\sigma(t) = G^*(\omega)\epsilon(t) = \epsilon_0|G^*(\omega)|e^{i(\omega t+\delta(\omega)}. \tag{1.1.1}$$

- If we denote $G(\infty) = \lim_{t\to\infty} G(t)$ and write the relaxation function as $G(t) = \Delta G(t) + G(\infty)$, complex modulus can be expressed as

$$G^*(\omega) = G(\infty) + i\omega \int_0^\infty \Delta G(s) e^{-i\omega s} ds.$$

- There is more direct way how to determine $G^*(\omega)$. Let us write the constitutive equation in the form

$$P(D)\sigma = Q(D)\epsilon,$$

where $P(x)$,$Q(x)$ are polynomials and $D$ is a symbolic time derivative. It can be shown that

$$G^*(\omega) = \frac{Q(i\omega)}{P(i\omega)}.$$

**Complex compliance**

In the same manner, let us consider a material subjected to oscillatory stress history

$$\sigma(t) = \sigma_0 e^{i\omega t}.$$

After a sufficient long time, the appropriate strain response becomes sinusoidal and if we expect it in a form

$$\epsilon(t) = \epsilon_c(t) + i\epsilon_s(t),$$

there again exist a function - complex compliance $J^*(\omega)$ such as

$$\epsilon(t) = J^*(\omega)\sigma(t),$$

which again can be expressed in the polar form

$$J^*(\omega) = |J^*(\omega)| e^{-i\alpha(\omega)}.$$

Complex functions $J^*(\omega)$ and $G^*(\omega)$ are coupled by the relation

$$J^*(\omega) = \frac{1}{G^*(\omega)}, \tag{1.1.2}$$

hence it can be also determined directly from a constitutive relation (using the notation from the previous page) by

$$J^*(\omega) = \frac{P(i\omega)}{Q(i\omega)}.$$

## Overview of models

There are several sets of material coefficients, especially in the case of Oldroyd model. Therefore we present it in the two most common variants. Regarding the identity (1.1.2), it holds

$$|J^*(\omega)| = \frac{1}{|G^*(\omega)|} \quad \text{and} \quad \alpha(\omega) = \delta(\omega).$$

Thus we do not show graphs of $|J^*(\omega)|$ and $\alpha(\omega)$ because it seems to be redundant. The graphs are prepared in the software Mathematica, the script is attached on CD.

Table 1.1: Table of material constants.

| | |
|---|---|
| $k$ | stiffness |
| $\nu, \nu_1, \nu_2$ | viscosities |
| $\lambda_1 = \frac{\nu}{E}$ | relaxation time for Maxwell and Oldroyd |
| $\lambda_2 = \frac{\nu_1 \nu_2}{k(\nu_1+\nu_2)}$ | retardation time for Oldroyd |
| $\eta = \nu_1 + \nu_2$ | zero shear viscosity for Oldroyd |

**Maxwell model**

$$\frac{\dot{\sigma}}{k} + \frac{\sigma}{\nu} = \dot{\epsilon}$$

$$G^*(\omega) = \frac{k\lambda_1^2\omega^2}{1+\lambda_1^2\omega^2} + i\frac{k\lambda_1\omega}{1+\lambda_1^2\omega^2}$$

$$J^*(\omega) = \frac{1}{k} - i\frac{1}{k\lambda_1\omega}$$

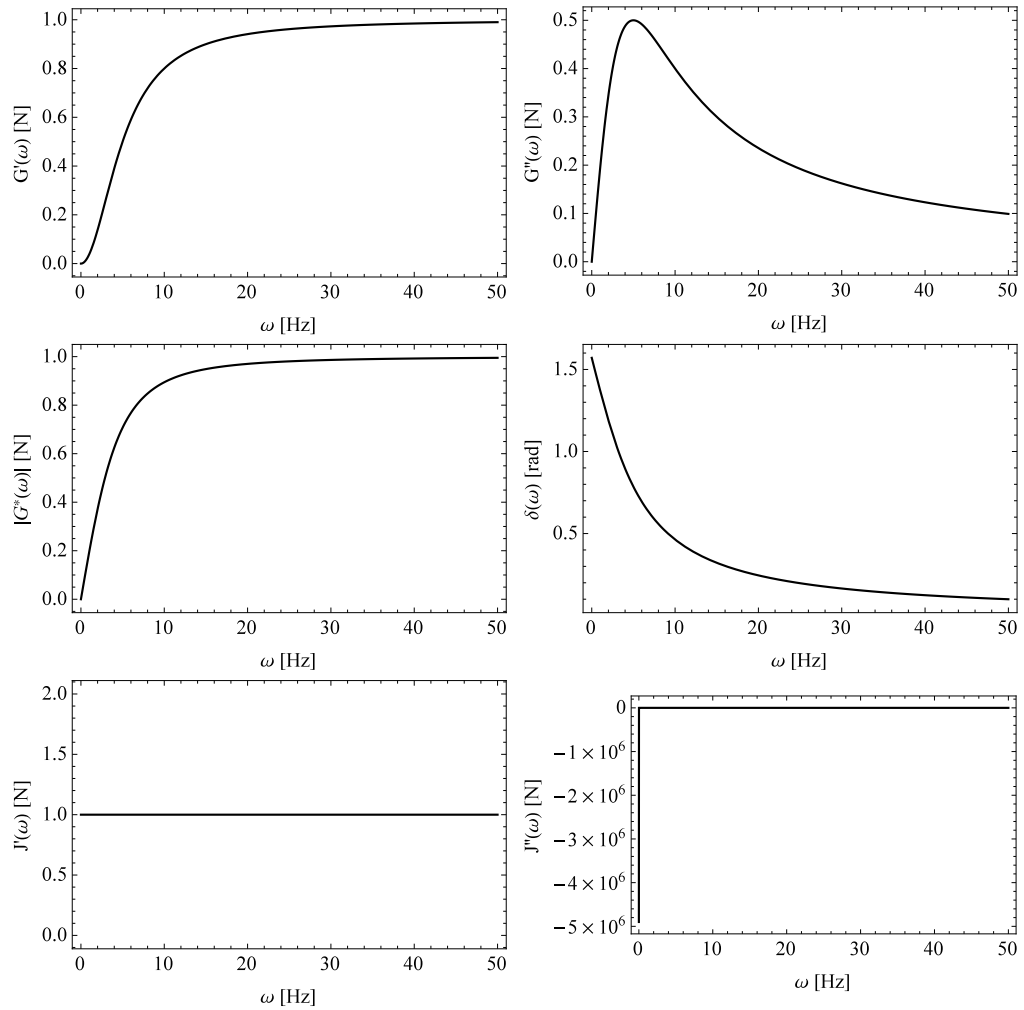



Figure 1.1: The dependence of complex modulus of the Maxwell model on frequency.

**Kelvin-Voigt model**

$$\sigma = \nu\dot{\epsilon} + k\epsilon$$

$$G^*(\omega) = k + ik\lambda_1\omega$$

$$J^*(\omega) = \frac{1}{k + k\lambda_1^2\omega^2} - i\frac{\lambda_1\omega}{k + k\lambda_1^2\omega^2}$$

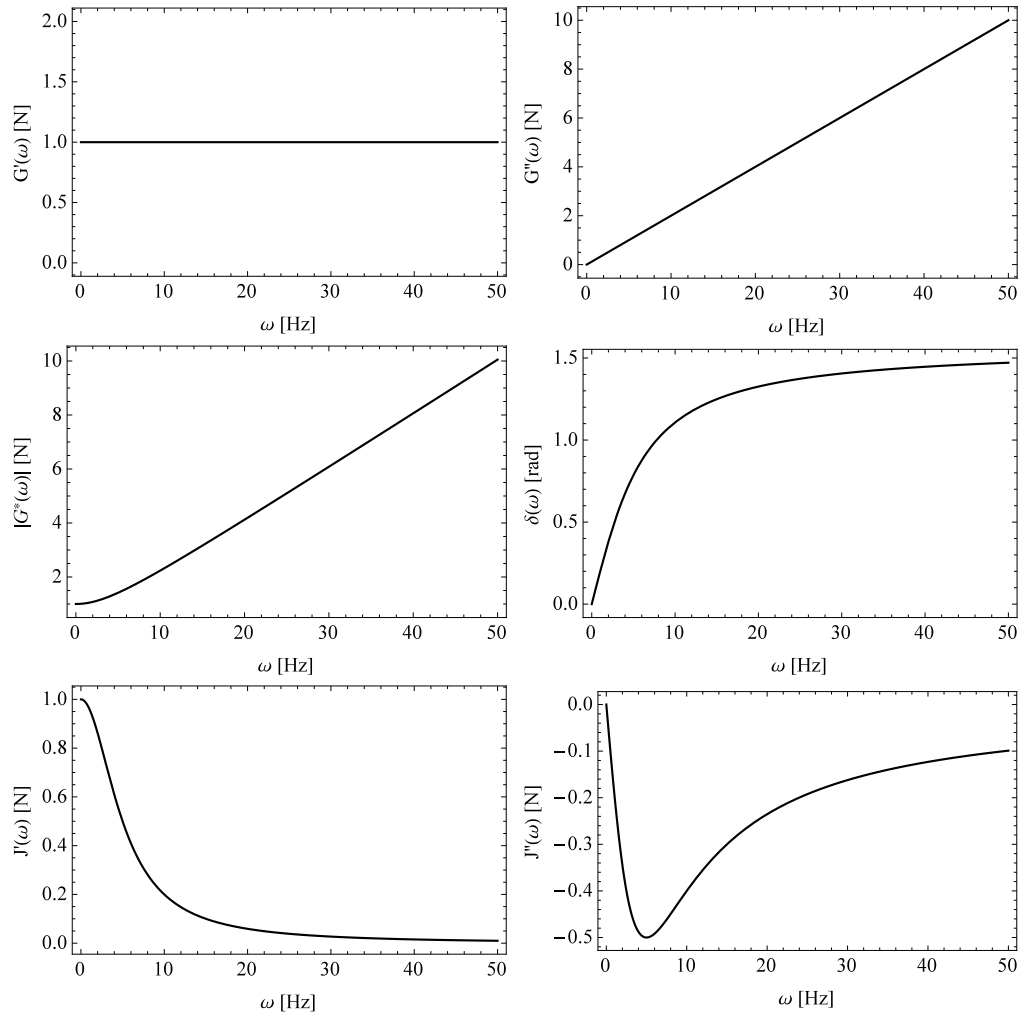



Figure 1.2: The dependence of complex modulus of the Kelvin-Voigt model on frequency.

**Oldroyd model**

$$\frac{\nu_1}{k}\dot{\sigma} + \sigma = (\nu_1 + \nu_2)\dot{\epsilon} - \frac{\nu_1\nu_2}{k}\ddot{\epsilon}$$

$$\lambda_1\dot{\sigma} + \sigma = \eta(\dot{\epsilon} - \lambda_2\ddot{\epsilon})$$

$$G^*(\omega) = \eta\omega^2\frac{(\lambda_1 - \lambda_2)}{1 + \lambda_1^2\omega^2} + i\eta\omega\frac{1 + \lambda_1\lambda_2\omega^2}{1 + \lambda_1^2\omega^2}$$

$$J^*(\omega) = \frac{\lambda_1 - \lambda_2}{\eta(1 + \lambda_2^2\omega^2)} - i\frac{1 + \lambda_1\lambda_2\omega^2}{\eta\omega(1 + \lambda_2^2\omega^2)}$$

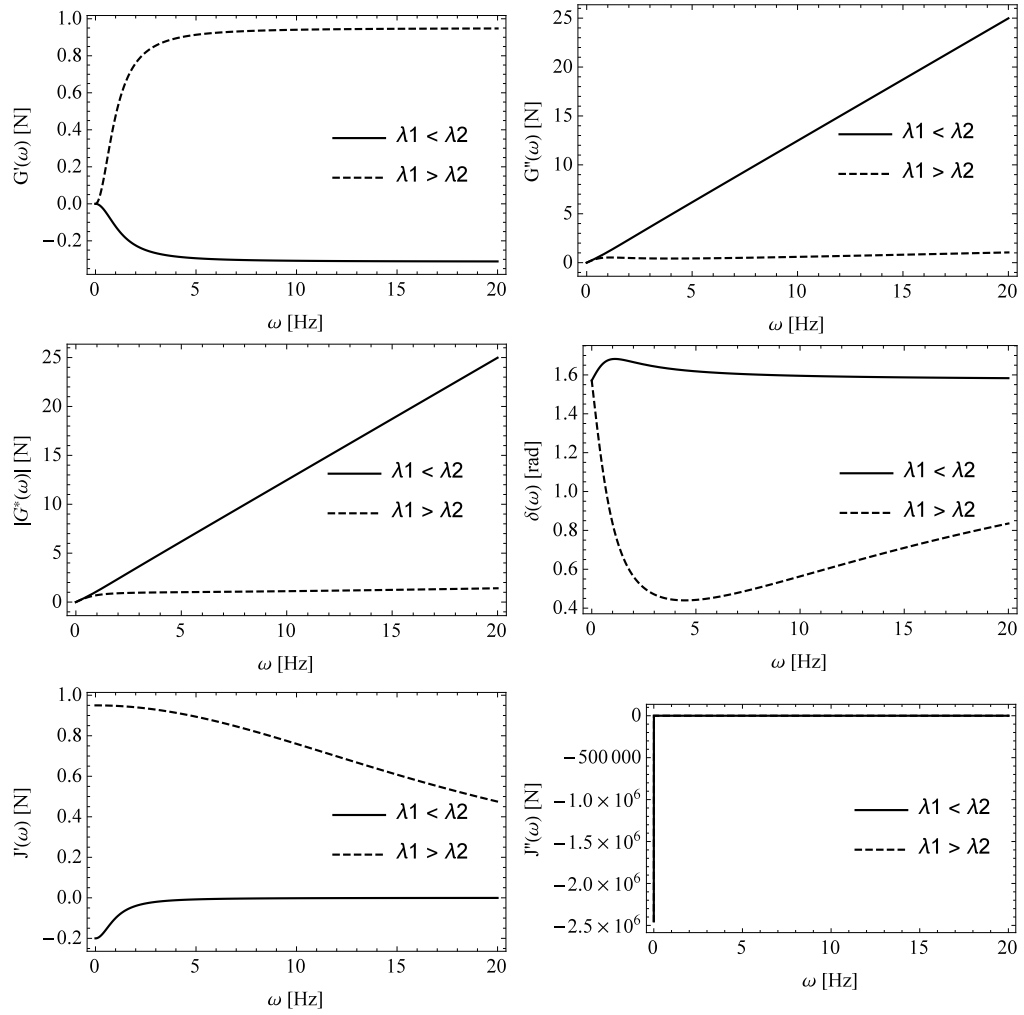



Figure 1.3: The dependence of complex modulus of the Oldroyd model on frequency. There are two types of curves, first for $\lambda_1 < \lambda_2$ (e. g. for $(\lambda_1, \lambda_2, \nu) = (0.8, 2, 1)$) and the second for $\lambda_1 > \lambda_2$ (e. g. for $(\lambda_1, \lambda_2, \nu) = (1, 0.5, 1)$. Material parametr $\eta$ only scales the graph and makes no difference in the shape.

**Burgers model**

$$\frac{\nu_1\nu_2}{k_1k_2}\ddot{\sigma} + (\frac{\nu_1}{k_2} + \frac{\nu_2}{k_2} + \frac{\nu_1}{k_1})\dot{\sigma} + \sigma = \frac{\nu_1\nu_2}{k_1}\ddot{\epsilon} + \nu_1\dot{\epsilon}$$

$$A\ddot{\sigma} + B\dot{\sigma} + \sigma = C\ddot{\epsilon} + D\dot{\epsilon}$$

$$G^*(\omega) = \frac{\omega^2(AC\omega^2 + BD - C)}{(1 - A\omega^2)^2 + B^2\omega^2} + i\frac{BC\omega^3 - AD\omega^3 + D\omega}{(1 - A\omega^2)^2 + B^2\omega^2}$$

$$J^*(\omega) = \frac{BD + C(A\omega^2 - 1)}{D^2 + C^2\omega^2} - i\frac{D + BC\omega^2 - AD\omega^2}{D^2\omega + C^2\omega^3}$$

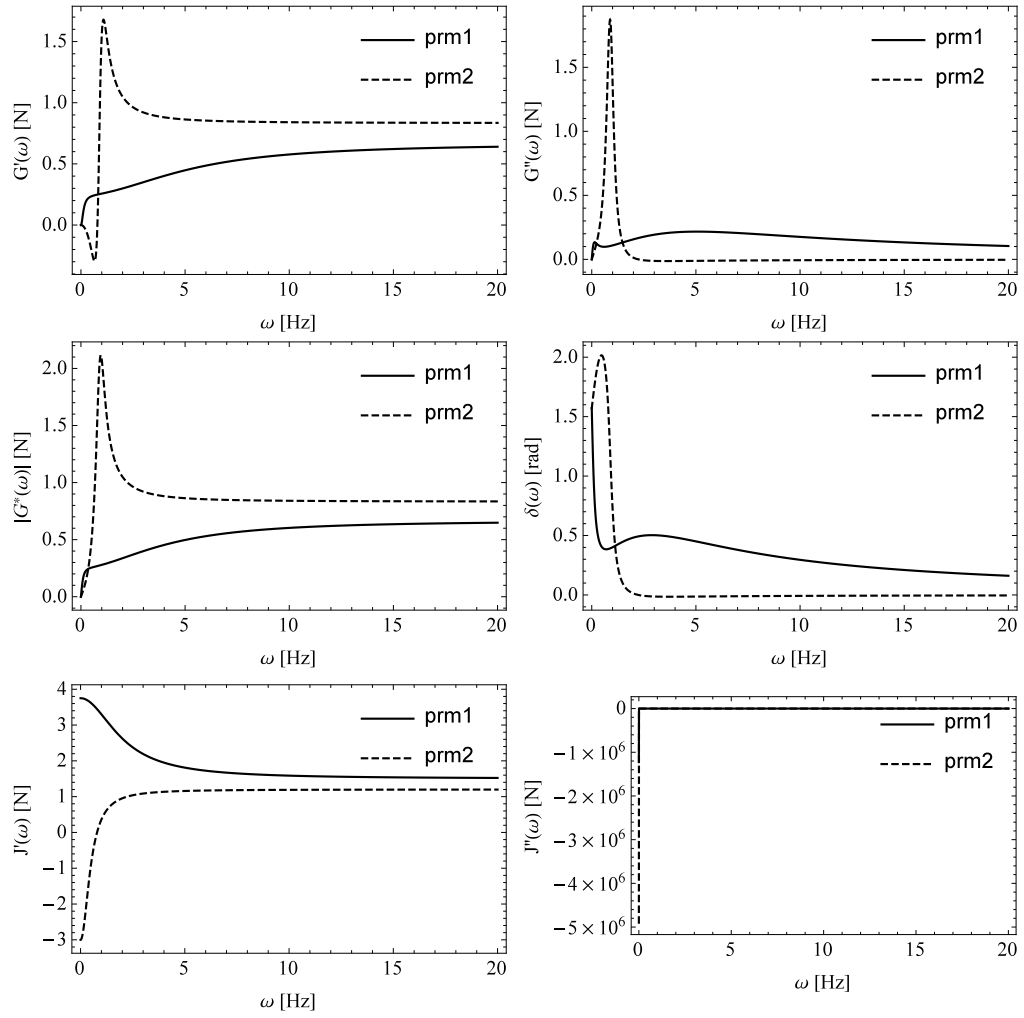



Figure 1.4: The dependence of complex modulus of the Burgers model on frequency. Graphs are plotted for two sets of material parameters $(A, B, C, D)$, prm1 $= (1.5, 8, 1, 2)$ and prm2 $= (1.2, 0.5, 1, 0.5)$ .

## 1.2 The Influence of the Temperature

Now we want to consider the influence of temperature $\theta$ via dependent material coefficients $\nu = \nu(\theta)$ and $k = k(\theta)$. We take the system of springs and dashpots

from the thermodynamic point of view, define thermodynamic quantities and we get the evolution equation for the temperature $\theta$. The derivation is rigorous, although it has no proper connection to the real materials. It is a rather an instrument for getting some intuition - how different models behaves under the temperature influence.

### 1.2.1 Springs and Dashpots as a Thermodynamic System

Let us consider a system of linear mechanical analogues with temperature dependent coefficients which consists of $k$ springs and $l$ dahspots. We have the constitutive relation for a spring

$$\sigma_i^{el} = k_i(\theta)\epsilon_i^{el}, \quad \text{for } i = 1, \dots, k \tag{1.2.1}$$

and for some stiffness functions $k_i(\theta)$ and for a dashpot

$$\sigma_i^{dis} = \nu_i(\theta)\dot{\epsilon_i^{dis}}, \quad \text{for } i = 1, \dots, l \tag{1.2.2}$$

and for some viscosity functions $\nu_i(\theta)$. From the physical reasons we assume $\nu_i(\theta)$ and $k_i(\theta)$ are non-increasing. Further we denote $\sigma$ and $\epsilon$ as total stress and total strain of the system, respectively. The assumption is there is a constant temperature $\theta$ in the whole system. It can be modelled by putting all mechanical analogues into a bath of fluid with infinity heat conduction coefficient.
Let us start the thermodynamic part with defining the free energy of the system

$$F(\theta, \epsilon_i^{el}) = F_0(\theta) + \sum_{i=1}^{k} \frac{k_i(\theta)}{2}(\epsilon_i^{el})^2 \tag{1.2.3}$$

with its thermodynamic part and mechanical one. We proceed by calculating entropy of the system using the identity

$$S(\theta, \epsilon_i^{el}) = -\frac{\partial F(\theta, \epsilon_i^{el})}{\partial \theta} = -\frac{\mathrm{d}F_0(\theta)}{\mathrm{d}\theta} - \sum_{i=1}^{k} \frac{\mathrm{d}k_i(\theta)}{\mathrm{d}\theta}\frac{1}{2}(\epsilon_i^{el})^2$$

and its time derivative

$$\dot{S(\theta, \epsilon_i^{el})} = \frac{\partial S(\theta, \epsilon_i^{el})}{\partial \theta}\dot{\theta} + \sum_{i=1}^{k} \frac{\partial S(\theta, \epsilon_i^{el})}{\partial \epsilon_i^{el}}\dot{\epsilon_i^{el}} = \frac{c_V}{\theta}\dot{\theta} - \sum_{i=1}^{k} \frac{\mathrm{d}k_i(\theta)}{\mathrm{d}\theta}\epsilon_i^{el}\dot{\epsilon_i^{el}}, \tag{1.2.4}$$

if we define $c_V$ in the standard way (although the subscript $V$ has no meaning in the system, where in fact no volume is considered). Considering Legendre transform $F = U - \theta S$, where $U$ denotes the total energy of the system, and using chain rule

$$\dot{F(\theta, \epsilon_i^{el})} = \frac{\partial F}{\partial \theta}\dot{\theta} + \sum_{i=1}^{k} \frac{\mathrm{d}F}{\mathrm{d}\epsilon_i^{el}}\dot{\epsilon_i^{el}}$$

we obtain

$$\theta\dot{S} = \dot{U} - \sum_{i=1}^{k} \frac{\mathrm{d}F}{\mathrm{d}\epsilon_i^{el}}\dot{\epsilon_i^{el}}.$$

Together with 1.2.4 it leads to

$$c_V\dot{\theta} = \dot{U} - \sum_{i=1}^{k}\left(\frac{\mathrm{d}F}{\mathrm{d}\epsilon_i^{el}} - \theta\frac{\partial^2 F}{\partial\theta\partial\epsilon_i^{el}}\right)\dot{\overline{\epsilon_i^{el}}} = \dot{U} - \sum_{i=1}^{k}\left(k_i(\theta) - \theta k_i'(\theta)\right)\epsilon_i^{el}\dot{\overline{\epsilon_i^{el}}}, \tag{1.2.5}$$

if we denote $k_i'(\theta) = \frac{\mathrm{d}k_i(\theta)}{\mathrm{d}\theta}$. Now we need to know something about the evolution of total energy $U$. This piece of information comes from the first law of thermodynamics

$$\mathrm{d}U = \delta Q + \delta W,$$

where $\delta Q$ denotes the infinitesimal increment of heat supplied to the system from its surroundings and $W$ infinitesimal increment of work done on the system. In our case, the work increment reads

$$\delta W = \sigma \mathrm{d}\epsilon.$$

Taking derivative leads to the balance of internal energy in the form

$$\dot{U} = r + \sigma\dot{\epsilon},$$

if we denote $\dot{Q} = r$ as a rate of heat flux.

Finally, we can substitute $\dot{U}$ to 1.2.5 and get the temperature evolution equation

$$c_V\dot{\theta} = \sigma\dot{\epsilon} - \sum_{i=1}^{k}\left(k_i(\theta) - \theta k_i'(\theta)\right)\epsilon_i^{el}\dot{\overline{\epsilon_i^{el}}} + r. \tag{1.2.6}$$

It can be written in the form

$$c_V\dot{\theta} = \left(\sigma\dot{\epsilon} - \sum_{i=1}^{k}\sigma_i^{el}\dot{\overline{\epsilon_i^{el}}}\right) + \sum_{i=1}^{k}\theta k_i'(\theta)\epsilon_i^{el}\dot{\overline{\epsilon_i^{el}}} + r, \tag{1.2.7}$$

where we can see the part of the mechanical energy stored within the springs, the part which does not turn into heat and hence does not contribute to the increment of the temperature.

### 1.2.2 Temperature dependent Models

Constitutive relation for temperature dependent models can differ from the classical ones. For example, it seen from the derivation for Maxwell model. We denote it T-Maxwell model to emphasise the difference. Next model presented here is T-Kelvin-Voigt. These are the simplest linear viscoelastic models, but we can demonstrate different behaviour of fluid-like model (T-Maxwell) and solid-like one (T-Kelvin-Voigt).

#### T-Maxwell model

$$\dot{\epsilon} = \frac{\sigma}{\nu(\theta)} + \frac{\dot{\sigma}}{k(\theta)} - \dot{\theta}\frac{\sigma k'(\theta)}{k^2(\theta)}, \tag{1.2.8a}$$

$$c_V\dot{\theta} = \frac{\sigma^2}{\nu(\theta)} - (k(\theta) - \theta k'(\theta))\frac{\sigma}{k(\theta)}\left(\dot{\epsilon} - \frac{\sigma}{\nu(\theta)}\right) + r \tag{1.2.8b}$$

**Derivation:** In derivation of the model, 1.2.8 we proceed as in the classical case. Due to the geometry, it holds

$$\epsilon = \epsilon^{dis} + \epsilon^{el} \quad \text{and} \quad \sigma = \sigma^{dis} = \sigma^{el}.$$

From 1.2.1, we have

$$\epsilon^{el} = \frac{\sigma}{k(\theta)},$$

hence

$$\dot{\epsilon^{el}} = \frac{\dot{\sigma}k(\theta) - \sigma k'(\theta)\dot{\theta}}{k^2(\theta)}$$

Similarly from 1.2.2 we have

$$\dot{\epsilon^{dis}} = \frac{\sigma}{\nu(\theta)}.$$

All together leads to

$$\dot{\epsilon} = \dot{\epsilon^{dis}} + \dot{\epsilon^{el}} = \frac{\sigma}{\nu(\theta)} + \frac{\dot{\sigma}k(\theta) - \sigma k'(\theta)\dot{\theta}}{k^2(\theta)}.$$

For the considered geometry, we can rewrite the evolution equation for the temperature 1.2.7 as

$$c_V\dot{\theta} = \sigma\dot{\epsilon^{dis}} - (k(\theta) - \theta k'(\theta))\epsilon^{el}\dot{\epsilon^{el}} + r.$$

Regarding the first term

$$\sigma\dot{\epsilon^{dis}} = \frac{\sigma^2}{\nu(\theta)}.$$

Further, $\dot{\epsilon^{el}} = (\dot{\epsilon} - \dot{\epsilon^{dis}})$ and using 1.2.2 and 1.2.1 leads to

$$\epsilon^{el}\dot{\epsilon^{el}} = \frac{\sigma}{k(\theta)}\left(\dot{\epsilon} - \frac{\sigma}{\nu(\theta)}\right) + r.$$

**T-Kelvin-Voigt model**

$$\sigma = \nu\dot{\epsilon} + k\epsilon \tag{1.2.9a}$$

$$c_V\dot{\theta} = \nu(\theta)(\dot{\epsilon})^2 - (k(\theta) - \theta k'(\theta))\epsilon\dot{\epsilon} + r \tag{1.2.9b}$$

**Derivation:** From the geometry of the model, we have

$$\epsilon = \epsilon^{dis} = \epsilon^{el} \quad \text{and} \quad \sigma = \sigma^{dis} + \sigma^{el}$$

and together with (from 1.2.1 and 1.2.2)

$$\sigma^{dis} = \nu(\theta)\epsilon^{dis},$$
$$\sigma^{el} = k(\theta)\epsilon^{el}$$

we can conclude that

$$\sigma = \nu(\theta)\epsilon + k(\theta)\epsilon^{el}.$$

Regarding the geometry, we can rewrite the evolution equation for the temperature 1.2.7 as

$$c_V\dot{\theta} = \sigma^{dis}\dot{\epsilon} - (k(\theta) - \theta k'(\theta))\epsilon\dot{\epsilon} + r,$$

which directly (using 1.2.2) leads to

$$c_V\dot{\theta} = \nu(\theta)(\dot{\epsilon})^2 - (k(\theta) - \theta k'(\theta))\epsilon\dot{\epsilon} + r.$$

### 1.2.3 Temperature Dependent Simulations

We compare these two models by considering sinusoidal stress

$$\sigma = sin(\omega t)$$

with frequency $\omega$. Then we solve the system of ordinary differential equations by Runge-Kutta method using function *DSolve[]* in the Mathematica software. Initial conditions are

$$\epsilon(0) = 0,$$
$$\theta(0) = 273.$$

Material functions are described by a triplets $\vec{k} = (k_1, k_2, k_3)$ and $\vec{\nu} = (\nu_1, \nu_2, \nu_3)$ and have the exponential form

$$k(\theta) = k_1 + k_2 e^{k_3(\theta - \theta_R)},$$
$$\nu(\theta) = \nu_1 + \nu_2 e^{\nu_3(\theta - \theta_R)},$$

where $\theta_R = 273$ is the reference temperature. Further we set $r = 0$ and $cV = 1$.

Figure 1.5 shows relatively steady state of the system. Note the fact that both systems are cooled by elongation. It is possible due to the second term on the right hand side in evolution equation of temperature (of both models 1.2.8 and 1.2.9), despite one would intuitively say that elongation of this system must cause an increment of temperature. We can observe this effect with real elastic rubber when we stretch it strong enough end apply to lips.

Figure 1.6 shows that T-Maxwell diverges (in the sense of temperature gain) if we fix $k = \text{konst}$. In the Figure 1.7 we fix $\nu = \text{konst}$ and observe an interesting shape of the strain response of the T-Maxwell model.

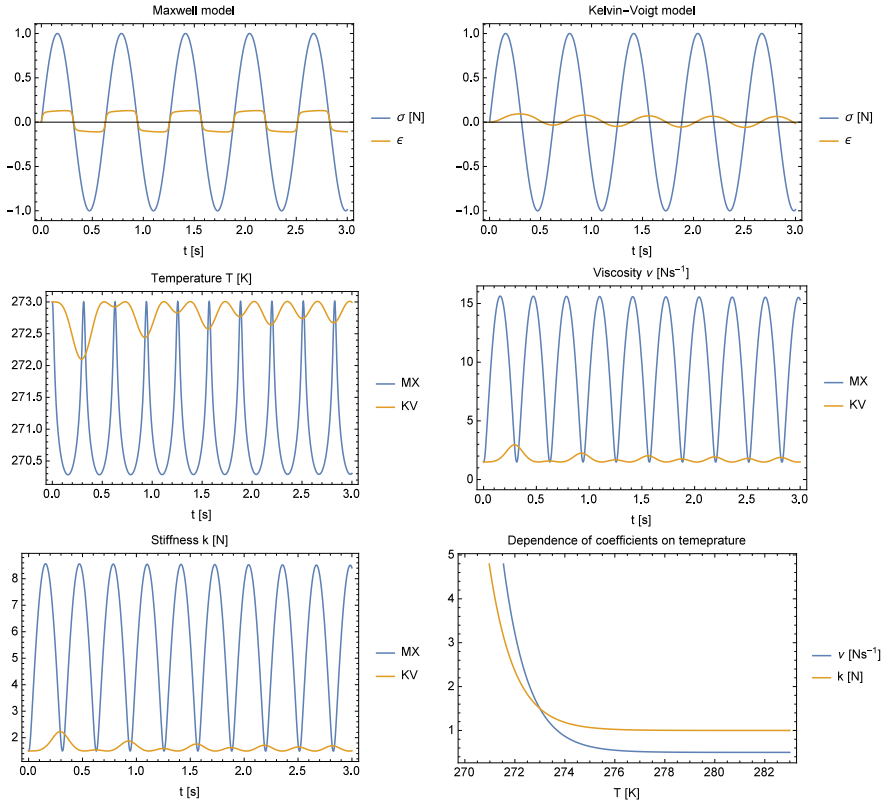



Figure 1.5: Comparison of models T-Maxwell (MX) and T-Kelvin-Voigt (KV) for parameters $\vec{k} = (1, 0.5, -1)$ and $\vec{\nu} = (0.5, 1, -1)$ and frequency $\omega = 10$Hz.

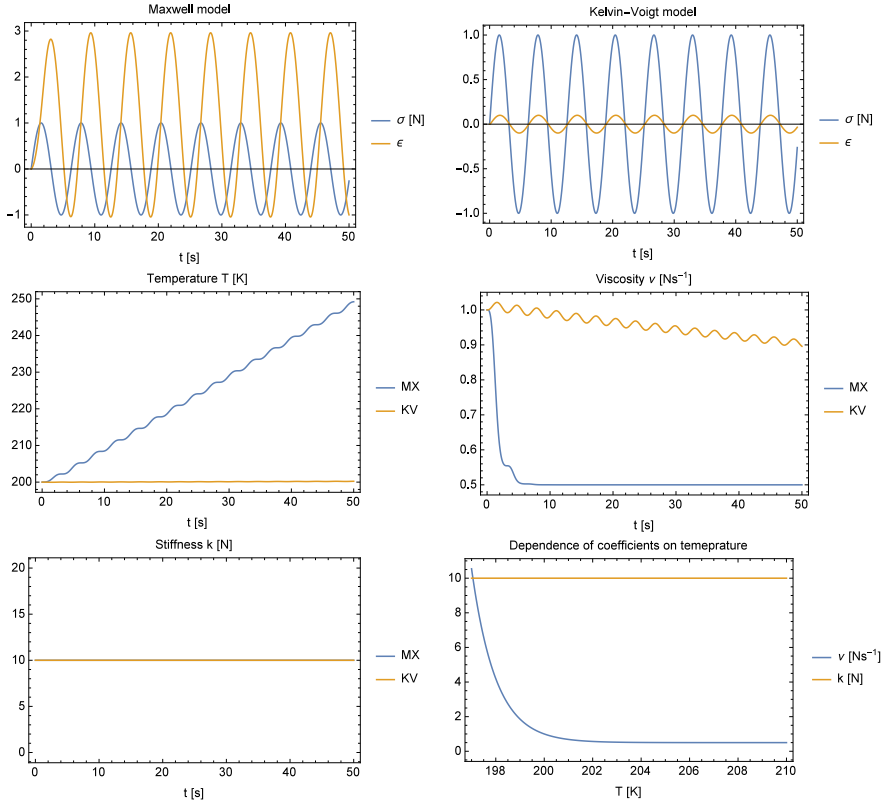



Figure 1.6: Comparison of models T-Maxwell (MX) and T-Kelvin-Voigt (KV) for parameters $\vec{k} = (10, 0, 0)$ and $\vec{\nu} = (0.5, 0.5, -1)$ and frequency $\omega = 1$Hz.

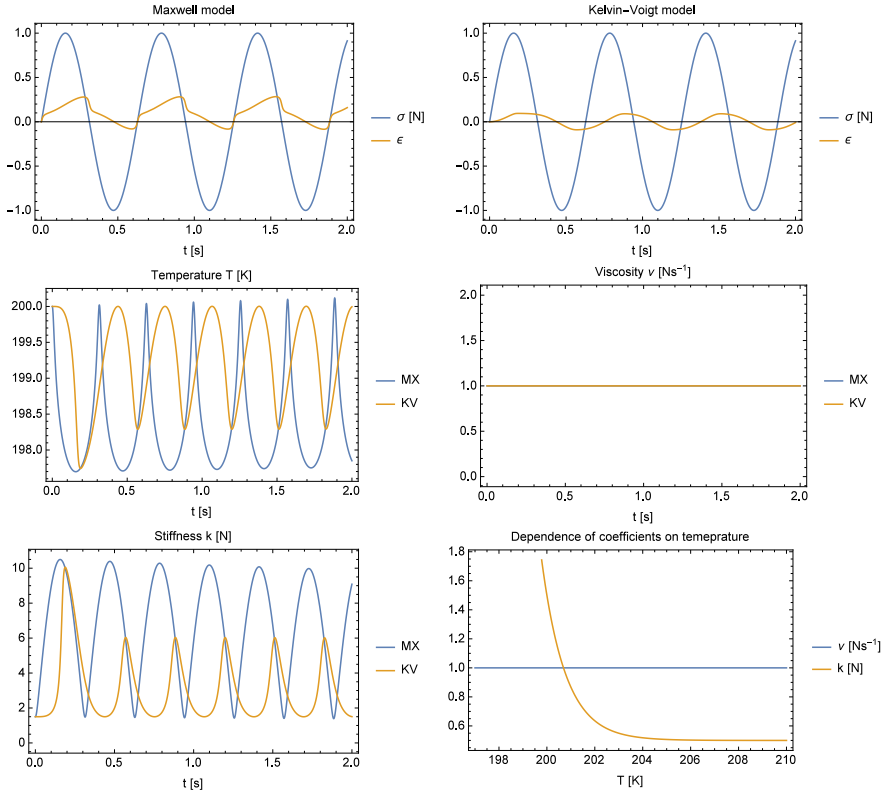



Figure 1.7: Comparison of models T-Maxwell (MX) and T-Kelvin-Voigt (KV) for parameters $\vec{k} = (0.5, 1, -1)$ and $\vec{\nu} = (1, 0, 0)$ and frequency $\omega = 10$Hz.

# 2. Constitutive Theory

## 2.1 Continuum Mechanics

If one wants to describe mechanical or kinematic properties of a body with continuous mass [1], continuum mechanics can be used. We assume the reader is familiar with the notion of continuum mechanics hence this section gives only a brief overview of basic notation used in this thesis. For more details about see any book concerning continuum mechanics, i.e. [9].

### 2.1.1 Basic Notation

Let us consider a continuous material body $\mathcal{B}$. In the following we proceed in the same way as in [15]. In a standard manner we define *reference configuration* $\kappa_R(\mathcal{B})$ and *present configuration* $\kappa_t(\mathcal{B})$ of the body.
Let $X \in \kappa_R$ and $x \in \kappa_t$ denote the material point $P \in \mathcal{B}$ at the reference and present configuration, respectively. Then we can define the *motion* $\chi_{\kappa_R}$ of the body as one-to-one mapping

$$x = \chi_{\kappa_R}(X, t).$$

Assuming its sufficient smoothness allows us to define the *velocity* $\hat{\mathbf{v}}$ as

$$\hat{\mathbf{v}}(X, t) = \frac{\partial \chi_{\kappa_R}(X, t)}{\partial t}$$

and the *acceleration* $\hat{\mathbf{a}}$ as

$$\hat{\mathbf{a}}(X, T) = \frac{\partial \hat{\mathbf{v}}(X, T)}{\partial t}$$

in Lagrangian (material) description. For our purpose it will be more useful to define the these quantities in Eulerian (spatial) description (for fixed $x$). Hence we have the *velocity*

$$\mathbf{v}(x, t) = \hat{\mathbf{v}}(\chi_{\kappa_R}^{-1}(x, t), t)$$

and the *acceleration*

$$\mathbf{a}(x, t) = \dot{\mathbf{v}} = \frac{\mathrm{d}\mathbf{v}(x, t)}{\mathrm{d}t} = \frac{\partial \mathbf{v}}{\partial t} + \frac{\partial \mathbf{v}(x, t)}{\partial x_i}\frac{\partial x_i}{\partial t} = \frac{\partial \mathbf{v}}{\partial t} + [\nabla \mathbf{v}]\mathbf{v},$$

where Einstein's summation convention is employed. In addition, the material time derivative for arbitrary quantity (scalar, vector of tensor) $s$ reads

$$\dot{s} = \frac{\mathrm{d}s}{\mathrm{d}t} = \frac{\partial s}{\partial t} + [\nabla s]\mathbf{v}.$$

Furthermore, we define the *deformation gradient*

$$\mathbf{F}_{\kappa_R} = \frac{\partial \chi_{\kappa_R}}{\partial X}, \quad (\text{or component-wise } \mathbf{F}_{\kappa_R}{}^{i}{}_{j} = \frac{\partial \chi^{i}_{\kappa_R}}{\partial X^{j}})$$

[1] In fact nothing consists of continuous mass but it is a sufficient approximation for spatial scales much greater than the size of atom or molecule.

and *left* and *right Cauchy-Green tensor*

$$\mathbf{B}_{\kappa_R} = \mathbf{F}_{\kappa_R}\mathbf{F}^T_{\kappa_R},\ \mathbf{C}_{\kappa_R} = \mathbf{F}^T_{\kappa_R}\mathbf{F}_{\kappa_R},$$

respectively. By direct calculation the *velocity gradient* is equal to

$$\mathbf{L} := \nabla\mathbf{v} = \dot{\mathbf{F}}_{\kappa_R}\mathbf{F}^{-1}_{\kappa_R},$$

the *symmetric part of the velocity gradient* is denoted by

$$\mathbf{D} = \frac{1}{2}(\mathbf{L} + \mathbf{L}^T)$$

and the *antisymmetric part of the velocity gradient* by

$$\mathbf{W} = \frac{1}{2}(\mathbf{L} - \mathbf{L}^T).$$

### 2.1.2 Balance Equations

In the previous the motion (deformation) $\chi_R(X,t)$ was a *given* function. Now we are interested in the question how to compute this function and the evolution of associated fields such as e.g. density and temperature. A standard way dealing with this issue is postulating general local balance equation for any quantity associated with the body $\mathcal{B}$ of single-component continuum. Let us consider a quantity $\mathcal{G}$ and its density $\gamma(x,t)$ associated with a spatial point $x$ in a time $t$ in Eulerian description [2]. There are three admissible mechanisms changing the value of $\gamma(x,t)$ in some control volume $\Omega_t$ [3], and their corresponding densities are

- production $\pi(x,t)$ of $\gamma$ inside $\Omega_t$,
- supply $\zeta(x,t)$ of $\gamma$ from outside of $\Omega_t$,
- flux $\mathbf{\Phi}(x,t)$ of $\gamma$ across the boundary $\partial\Omega_t$ of $\Omega_t$.

Hence a balance of $\gamma$ in $\Omega_t$ reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_t}\gamma\,\mathrm{dv} = -\int_{\partial\Omega_t}\mathbf{\Phi}\,\mathrm{dS} + \int_{\Omega_t}\pi\,\mathrm{dv} + \int_{\Omega_t}\zeta\,\mathrm{dv}.$$

Using Reynolds transport theorem, Gauss theorem and localization, the general local balance equation (for a scalar, vector or tensor quantity) then can be written as

$$\frac{\mathrm{d}\gamma}{\mathrm{d}t} + \gamma\,\mathrm{div}\,\mathbf{v} = -\mathrm{div}\,\mathbf{\Phi} + \pi + \zeta.$$

Now particular balance equations comes as a consequence of the general one by setting specific quantities.

[2] Detailed explanation and motivation for this approach with its assumptions can be found in [9].

[3] Control volume $\Omega_t$ is associated with a fixed set of material points therefore it changes in time.

### Mass balance

Setting

- density $\gamma^{\rho} = \rho(x,t)$, where $\rho$ denotes mass density (or simply "density"),
- production $\pi^{\rho} = 0$,
- supply $\zeta^{\rho} = 0$,
- flux $\mathbf{\Phi}^{\rho} = 0$,

we obtain mass balance (or also called *continuity equation*)

$$\dot{\rho} + \rho \operatorname{div} \mathbf{v} = 0. \tag{2.1.1}$$

For an incompressible case (which means $\det \mathbf{F} = \text{const} = 1$), this reduces to the condition

$$\operatorname{div} \mathbf{v} = 0. \tag{2.1.2}$$

### Momentum balance

If we set

- density $\gamma^{\rho v} = \rho \mathbf{v}$,
- production $\pi^{\rho v} = 0$,
- supply $\zeta^{\rho v} = \rho \mathbf{b}$, where $\mathbf{b}$ denotes outer body force,
- flux $\mathbf{\Phi}^{\rho v} = -\mathbf{T}$, where tensor $\mathbf{T}$ is the *Cauchy stress tensor*,

we can (using mass balance 2.1.1) obtain momentum balance in a form

$$\rho \dot{\mathbf{v}} = \operatorname{div} \mathbf{T} + \rho \mathbf{b}. \tag{2.1.3}$$

### Angular Momentum Balance

Making an assumption that the particles in body $\mathcal{B}$ do not have internal angular momentum (spin) and considering

- density $\gamma^{\rho x \times x} = x \times \rho \mathbf{v}$,
- production $\pi^{\rho x \times x} = 0$,
- supply $\zeta^{\rho x \times x} = x \times \rho \mathbf{b}$,
- flux $\mathbf{\Phi}^{\rho x \times x} = -x \times \mathbf{T}$,

we can show that angular momentum balance does not yield additional differential equation, but it implies symmetry condition for the Cauchy stress tensor

$$\mathbf{T} = \mathbf{T}^T. \tag{2.1.4}$$

**Energy Balance**

The first law of thermodynamics states that the mechanical and thermal energy (and all additional energies present) are not conserved individually but they are conserved together, hence we set

- density $\gamma^E = \frac{1}{2}\rho\mathbf{v}\cdot\mathbf{v} + \rho e$ , kinetic + internal energy,
- production $\pi^E = 0$,
- supply $\zeta^E = \rho\mathbf{b}\cdot\mathbf{v} + \rho r$, where $r$ denotes the density of energy sources,
- flux $\mathbf{\Phi}^E = -\mathbf{T}\mathbf{v} + \mathbf{q}$, where $\mathbf{q}$ is the energy flux,

to obtain total energy balance

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{2}\rho|\mathbf{v}|^2 + \rho e\right) + \left(\frac{1}{2}\rho|\mathbf{v}|^2 + \rho e\right)\mathbf{div}\,\mathbf{v} = \operatorname{div}\mathbf{T}\mathbf{v} - \operatorname{div}\mathbf{q} + \rho\mathbf{b}\cdot\mathbf{v} + \rho r.$$

Using mass balance 2.1.1 and momentum balance 2.1.3 we arrive at the *internal energy balance* in the form

$$\rho\dot{e} = \mathbf{T} : \mathbf{D} - \operatorname{div}\mathbf{q} + \rho r. \tag{2.1.5}$$

At this point we have three evolutionary differential equations (2.1.1, 2.1.3 and 2.1.5) for three unknowns $\rho$, $\mathbf{v}$ and $e$. These balance equations represent general laws independent of the chosen material. If outer sources ($r$ and $\mathbf{b}$) are set up, it remains to specify the material by providing constitutive relations for $\mathbf{T}$ and $\mathbf{q}$.

For example a standard viscous incompressible Navier-Stokes-Fourier (NSF) model (for more details about NSF model, see [17]) is defined by constitutive relation

$$\mathbf{T} = -p\mathbf{I} + 2\mu(\theta)\mathbf{D} \;\text{ and }\; \mathbf{q} = -k(\theta)\nabla\theta, \tag{2.1.6}$$

where $-p = \frac{1}{3}\operatorname{tr}\mathbf{T}$ is the mean normal stress and $\theta$ denotes thermodynamic temperature, $\mu(\theta)$ and $k(\theta)$ are temperature dependent material parameters (viscosity and thermal conductivity, respectively). In incompressible case, the mass balance 2.1.1 enforces only

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

and unknown $\rho$ becomes a parameter [4]. Therefore we can compute $p$ as additional unknown. On the other hand, in a compressible case, a special constitutive equation for $p = \tilde{p}(\rho)$ or $p = \tilde{p}(\rho,\theta)$ has to be prescribed.

Temperature $\theta$ is new unknown without an evolution equation. Hence our goal is to find a way how to rewrite energy balance as an temperature balance.

[4] Precisely speaking, it is true only in the case of homogeneous body. But in the case of heterogeneous body, density $\rho$ is still known due to fact, that its material time derivative remains zero. If initial density field $\rho(x,0)$ is given, we can obtain $\rho(x,t)$ at any time $t$ as $\rho(x,0)$ wafted by the motion.

The goal is achieved for an incompressible NSF model by postulating the internal energy in the form

$$e = c_v \theta,$$

where $c_v > 0$ is a heat capacity at constant volume.

In general, whenever dissipative processes are involved, the continuum mechanics framework must be extended for another quantity - entropy.

**Entropy Balance**

Considering entropy balance is important for fulfilling the second law of thermodynamics. Let us set

- density $\gamma^S = \rho\eta$
- production $\pi^S = \Xi$
- supply $\zeta^S = \rho\Upsilon$
- flux $\mathbf{\Phi}^S = \mathbf{\Psi}$

which leads to

$$\rho\dot{\eta} = -\operatorname{div} \mathbf{\Psi} + \Xi + \rho\Upsilon, \tag{2.1.7}$$

When developing a new material model, one must identify each contribution to the entropy balance and then guarantee $\Xi > 0$, so that the second law of thermodynamics would be satisfied.

### 2.1.3 Temperature Evolution Equation

In the same manner as in [4], let us assume the internal energy depends on density, entropy and other quantities, that is $e = \tilde{e}(\rho, \eta, y_1, y_2, ..., y_k)$, $k \in \mathbf{N}$, and define (positive) thermodynamic temperature as

$$\theta = \frac{\partial e}{\partial \eta}.$$

If we define the Helmholtz free energy $\psi = \tilde{\psi}(\rho, \theta, y_1, y_2, ..., y_k)$ using Legendre transform with respect to $\eta$

$$\psi = e - \theta\eta,$$

we can rewrite the balance equation for internal energy (2.1.5) as

$$\rho\dot{\psi} + \rho\dot{\theta}\eta + \rho\theta\dot{\eta} = \mathbf{T} : \mathbf{D} - \operatorname{div} \mathbf{q} + \rho r. \tag{2.1.8}$$

The free energy is dependent on density, temperature and other quantities, one can express its time derivative by the chain rule

$$\dot{\psi} = \frac{\partial\tilde{\psi}}{\partial\rho}\dot{\rho} + \frac{\partial\tilde{\psi}}{\partial\theta}\dot{\theta} + \sum_{i=1}^{k} \frac{\partial\tilde{\psi}}{\partial y_i} \cdot \dot{y}_i, \tag{2.1.9}$$

where a multiplication in the last term is chosen appropriate to the tensorial order of a parameter $y_i$. We proceed by known thermodynamic identities

$$\frac{\partial\tilde{\psi}}{\partial\rho} = \frac{p}{\rho^2} \text{ and } \frac{\partial\tilde{\psi}}{\partial\theta} = -\eta. \tag{2.1.10}$$

The first one can be understood as a definition of a thermodynamic pressure $p$. Finally, using (2.1.10), (2.1.9) and balance of mass (2.1.1), we can rewrite equation (2.1.8) as

$$\rho\theta\dot{\eta} = \mathbf{T} : \mathbf{D} - \operatorname{div}\mathbf{q} + p\operatorname{div}\mathbf{v} - \rho\sum_{i=1}^{k}\frac{\partial\tilde{\psi}}{\partial y_i}\cdot\dot{y}_i + \rho r \tag{2.1.11}$$

We would like to identify particular terms in (2.1.11) with terms in the general entropy balance (2.1.7). But it is not possible at this point because it depends on the form of the free energy $\tilde{\psi}$ (for example the term $\dot{y}_i$ can contribute to entropy flux). However, in classical thermodynamics entropy flux, entropy production and entropy supply are mostly used in a form

$$\mathbf{\Phi} = \frac{\mathbf{q}}{\theta}, \quad \Xi = \frac{\xi}{\theta}, \quad \Upsilon = \frac{r}{\theta},$$

where $\xi$ is called *rate of entropy production* [5]. This choice allows us to rewrite (2.1.11) as

$$\rho\dot{\eta} = -\operatorname{div}\frac{\mathbf{q}}{\theta} + \frac{1}{\theta}\left[\mathbf{T} : \mathbf{D} - \frac{\mathbf{q}\cdot\nabla\theta}{\theta} + p\operatorname{div}\mathbf{v} - \rho\sum_{i=1}^{k}\frac{\partial\tilde{\psi}}{\partial y_i}\cdot\dot{y}_i\right] + \rho\frac{r}{\theta}, \tag{2.1.12}$$

although it still can not be identified with general entropy balance.

We can go further to obtain evolution equation for the temperature. From (2.1.10) and chain rule we have

$$\eta = -\frac{\partial\tilde{\psi}(\rho,\theta,y_1,y_2,...,y_k)}{\partial\theta} = \tilde{\eta}(\rho,\theta,y_1,y_2,...,y_k),$$

$$\dot{\eta} = \frac{\partial\tilde{\eta}}{\partial\rho}\dot{\rho} + \frac{\partial\tilde{\eta}}{\partial\theta}\dot{\theta} + \sum_{i=1}^{k}\frac{\partial\tilde{\eta}}{\partial y_i}\cdot\dot{y}_i.$$

Using (2.1.10), smoothness of $\tilde{\psi}$, mass balance (2.1.1), another thermodynamic identities and definition of $c_V$ as a specific heat at a constant volume

$$\begin{aligned}
\dot{\rho}\frac{\partial\tilde{\eta}}{\partial\rho} = -\dot{\rho}\frac{\partial^2\tilde{\psi}}{\partial\rho\,\partial\theta} = -\dot{\rho}\frac{1}{\rho^2}\frac{\partial p}{\partial\theta} = \frac{1}{\rho}\frac{\partial p}{\partial\theta}\operatorname{div}\mathbf{v},\\
\frac{\partial\tilde{\eta}}{\partial\theta} = \frac{c_v}{\theta},\\
\frac{\partial\tilde{\eta}}{\partial y_i} = -\frac{\partial^2\tilde{\psi}}{\partial\theta\,\partial y_i},
\end{aligned}$$

one can rewrite (2.1.11) to the *temperature evolution equation* expressed as

$$\rho c_v\dot{\theta} = \mathbf{T} : \mathbf{D} - \operatorname{div}\mathbf{q} + (p - \theta\frac{\partial p}{\partial\theta})\operatorname{div}\mathbf{v} - \rho\sum_{i=1}^{k}(\frac{\partial\tilde{\psi}}{\partial y_i} - \theta\frac{\partial^2\tilde{\psi}}{\partial\theta\,\partial y_i})\cdot\dot{y}_i + \rho r. \tag{2.1.13}$$

[5] In a lot of literature, $\Xi$ is called rate of entropy production and $\xi$ is called rate of dissipation. But to be consisten for example with the doctoral thesis [15], we us the notation defined above.

## 2.2 Derivation of Temperature Dependent Viscoelastic Models

In order to derive thermodynamically consistent models, we use a thermodynamic framework proposed by Rajagopal and Srinivasa in 2000 [12]. This framework is based on a notion of natural configuration and the principle of maximal rate of entropy production (PMREP). In this section we introduce the framework and derive several incompressible viscoelastic models. In addition, we derive the viscous incompressible Navier-Stokes-Fourier model as an example. In this section, we denote $d = 2, 3$ as a geometric dimension of the problem.

### 2.2.1 Natural Configuration

In order to derive viscoelastic models we suppose the total deformation $\chi_{\kappa_R}$ is homogenous and can be divided into a purely elastic part and a purely dissipative part. Then one can consider a special configuration called *natural configuration* $\kappa_{p(t)}$ and state [6]

- the deformation $\chi_{dis} : \kappa_R \to \kappa_{p(t)}$ is purely dissipative (does not store energy)
- the deformation $\chi_{el} : \kappa_{p(t)} \to \kappa_t$ is purely elastic (does not dissipate energy).

Motivation for this concept is a need to capture microscopical changes in a material during a process. If there are more microscopical mechanisms within a material, one should consider multiple natural configuration to capture these mechanisms separately. For more details see [13].

All kinematics we have defined for the total deformation $\chi_R$ can be defined for the dissipative $\chi_{dis}$ and the elastic $\chi_{el}$ part. For a clarity in understanding, our notation is consistent with [13].

#### Elastic part

First we introduce *deformation gradient of the elastic part*

$$\mathbf{F}_{\kappa_p(t)} = \frac{\partial \chi_{el}(X_p, t)}{\partial X_p},$$

where $X_p \in \kappa_p(t)$ and $x = \chi_{el}(X_p, t) \in \kappa_t$ correspond to a material point $X$. We want to quantify the amount of energy stored during en elastic deformation, hence we introduce left and right Cauchy-Green tensors

$$\mathbf{B}_{\kappa_p(t)} = \mathbf{F}_{\kappa_p(t)}\mathbf{F}^T_{\kappa_p(t)}, \ \mathbf{C}_{\kappa_p(t)} = \mathbf{F}^T_{\kappa_p(t)}\mathbf{F}_{k_p(t)}.$$

[6] In general, it is not always possible to decompose the total deformation in two one-to-one mappings. But it can be done locally thus it is possible to define gradients of these mappings, and that is all we need. The gradients can be thought also as mappings from appropriate tangent spaces to the configuration manifolds.

### Dissipative part

To hold a consistency assumption let us denote *deformation gradient of the dissipative part* as $\mathbf{G}$ and it holds

$$\mathbf{G} = \mathbf{F}\mathbf{F}_{\kappa_p(t)}^{-1}$$

and appropriate *velocity gradient of the dissipative part* by $\mathbf{L}_{\kappa_p(t)}$, which can be expressed by

$$\mathbf{L}_{\kappa_p(t)} = \dot{\mathbf{G}}\mathbf{G}^{-1}.$$

Finally a useful quantity to measure the rate of entropy production (dissipation) due to evolution of natural configuration is symmetric part of $\mathbf{L}_{\kappa_p(t)}$ denoted as

$$\mathbf{D}_{\kappa_p(t)} = \frac{1}{2}(\mathbf{L}_{\kappa_p(t)} + \mathbf{L}_{\kappa_p(t)}^T).$$

### Useful identities

As we will see it is important to know something about time evolution of a quantity connected with natural configuration. In our derivation this quantity is $\mathbf{B}_{\kappa_p(t)}$ and its material time derivative can be expressed as

$$\dot{\mathbf{B}}_{\kappa_p(t)} = \mathbf{L}\mathbf{B}_{\kappa_p(t)} + \mathbf{B}_{\kappa_p(t)}\mathbf{L}^T - 2\mathbf{F}_{\kappa_p(t)}\mathbf{D}_{\kappa_p(t)}\mathbf{F}_{\kappa_p(t)}^T. \tag{2.2.1}$$

Unfortunately, under observer transformation

$$\mathbf{x}^* = \mathbf{Q}(t)\mathbf{x} + \mathbf{c}(t), \quad \mathbf{Q}(t)\mathbf{Q}(t)^T = \mathbf{Q}(t)^T\mathbf{Q}(t) = \mathbf{I}$$

a material time derivative of a second order tensor is not objective (or frame indifferent)

$$\frac{\mathrm{d}\mathbf{A}^*}{\mathrm{d}t} = \dot{\mathbf{Q}}\mathbf{A}\mathbf{Q}^T + \mathbf{Q}\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t}\mathbf{Q}^T + \mathbf{Q}\mathbf{A}\dot{\mathbf{Q}}^T \neq \mathbf{Q}\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t}\mathbf{Q}^T.$$

Introducing the upper convected Oldroyd time derivative

$$\overset{\triangledown}{A} := \frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t} - \mathbf{L}\mathbf{A} - \mathbf{A}\mathbf{L}^T$$

as the objective material time derivative, we can rewrite 2.2.1 as

$$\overset{\triangledown}{\mathbf{B}}_{\kappa_p(t)} = -2\mathbf{F}_{\kappa_p(t)}\mathbf{D}_{\kappa_p(t)}\mathbf{F}_{\kappa_p(t)}^T. \tag{2.2.2}$$

It also holds

$$\overline{\dot{\mathrm{tr}\,\mathbf{B}_{\kappa_p(t)}}} = 2\mathbf{B}_{\kappa_p(t)} : \mathbf{D} - 2\mathbf{C}_{\kappa_p(t)} : \mathbf{D}_{\kappa_p(t)}, \tag{2.2.3}$$

$$\overline{\dot{\det\mathbf{B}_{\kappa_p(t)}}} = \det\mathbf{B}_{\kappa_p(t)}\mathbf{B}_{\kappa_p(t)}^{-T} : \dot{\mathbf{B}}_{\kappa_p(t)} = 2\mathbf{I} : \mathbf{D} - 2\mathbf{I} : \mathbf{D}_{\kappa_p(t)} \tag{2.2.4}$$

and

$$\overset{\triangledown}{\mathbf{I}} = -2\mathbf{D}.$$

### 2.2.2 Principle of Maximal Rate of Entropy Production

Considering natural configuration the total deformation is split into two parts. The elastic response is characterized by the choice of the free energy $\hat{\psi}$. Next step is defining the rate of entropy production $\hat{\xi}$ which describes mechanisms causing the dissipation of energy. We choose this so that it is non-negative to automatically satisfy the second law of thermodynamics.

At this point, PMREP is applied to obtain constitutive relations for $\mathbf{T}$ and $\mathbf{q}$. According to the principle, we should maximize the rate of entropy production $\hat{\xi}$ with respect to constraint $\hat{\xi} = \xi$. Motivation for maximization of the rate of entropy production can be found in [14]. If we assume dissipative or elastic (or both) part incompressible, we should also consider additional constraints. By a triple ([IC]3) let us denote (in)compressibility of the total deformation, the dissipative part and the elastic part, respectively. The incompressibility conditions are detailed in [15], but in our thesis we are interested only in the cases, where the total deformation is incompressible. There are two possibilities.

- (III) fully incompressible case with constraints $\operatorname{tr}\mathbf{D} = 0$ and $\operatorname{tr}\mathbf{D}_{\kappa_{\mathbf{p}}(\mathbf{t})} = 0$,
- (ICC) both elastic and dissipative part are compressible with constraint $\operatorname{tr}\mathbf{D} = 0$ only for the total deformation.

The maximization is performed with aid of the method of Lagrange multipliers. Constitutive relations for $\mathbf{T}$, $\mathbf{q}$ and evolution equations for quantities $y_i$ come from the necessary conditions for the extreme (maximum).

### 2.2.3 Exemplary Derivation of Viscous Model

For better understanding of the framework, we show as an example derivation of well known incompressible Navier-Stokes-Fourier model. Let us assume a deformation of an incompressible Newtonian (non-elastic) fluid. The free energy of this material is

$$\hat{\psi} = \hat{\psi}_0(\rho, \theta).$$

Therefore, we can substitute $\hat{\psi}$ in 2.1.12, use the incompressibility condition $\operatorname{div}\mathbf{v} = 0$ and obtain

$$\rho\dot{\eta} = -\operatorname{div}\frac{\mathbf{q}}{\theta} + \frac{1}{\theta}\left[\mathbf{T} : \mathbf{D} - \frac{\mathbf{q}\cdot\nabla\theta}{\theta}\right] + \rho\frac{r}{\theta}.$$

Now we can compare the result with the general entropy balance 2.1.7 and identify the entropy flux $\mathbf{\Psi} = \frac{\mathbf{q}}{\theta}$, the entropy supply $\Upsilon = \frac{r}{\theta}$ and in particular the entropy production as

$$\xi = \mathbf{T} : \mathbf{D} - \frac{\mathbf{q}\cdot\nabla\theta}{\theta}.$$

Also from 2.1.13 we obtain evolution equation for the temperature as

$$\rho c_v\dot{\theta} = \mathbf{T} : \mathbf{D} - \operatorname{div}\mathbf{q} + \rho r.$$

Next step is defining the rate of entropy production. In this case, a suitable choice is the one for a standard viscous material

$$\hat{\xi}(\mathbf{D}, \nabla\theta) = 2\mu(\theta)\mathbf{D} : \mathbf{D} + \frac{k(\theta)}{\theta}\nabla\theta\cdot\nabla\theta,$$

where $\mu(\theta) \geq 0$ and $k(\theta) \geq 0$ denotes viscosity and heat conductivity, respectively. Since we are dealing with an incompressible material, we consider the case (III) (see subsection 2.2.2) with a trivial elastic part $\chi_{el}$, therefore $\chi_R = \chi_{dis}$ are identical, specially $\operatorname{tr}\mathbf{D} = \operatorname{tr}\mathbf{D}_{\kappa_p(t)}$, and constraints for maximization $\hat{\xi}(\mathbf{D}, \nabla\theta)$ are

$$\hat{\xi} = \xi \qquad \text{and} \qquad \operatorname{tr}\mathbf{D} = 0.$$

In order to find the necessary conditions for an extreme, we define the Lagrange function

$$L(\mathbf{D}, \nabla\theta) = \hat{\xi}(\mathbf{D}, \nabla\theta) - \lambda_1(\hat{\xi}(\mathbf{D}, \nabla\theta) - \xi) - \lambda_2(\operatorname{tr}\mathbf{D})$$

and after substitution

$$\begin{aligned} L(\mathbf{D}, \nabla\theta) = {} & 2\mu(\theta)\mathbf{D} : \mathbf{D} + \frac{k(\theta)}{\theta}\nabla\theta \cdot \nabla\theta \\ & - \lambda_1 \left( 2\mu(\theta)\mathbf{D} : \mathbf{D} + \frac{k(\theta)}{\theta}\nabla\theta \cdot \nabla\theta - \mathbf{T} : \mathbf{D} - \frac{\mathbf{q} \cdot \nabla\theta}{\theta} \right) - \lambda_2(\operatorname{tr}\mathbf{D}). \end{aligned}$$

Evaluating the partial derivatives of $L$ with respect to $\mathbf{D}$ and $\nabla\theta$ [7] and setting them to zero yields

$$0 = \frac{\partial L}{\partial \mathbf{D}} = 4\mu(\theta)\mathbf{D} - \lambda_1 \left(4\mu(\theta)\mathbf{D} - \mathbf{T}\right) - \lambda_2\mathbf{I}, \tag{2.2.5}$$

$$0 = \frac{\partial L}{\partial \nabla\theta} = 2\frac{k(\theta)}{\theta}\nabla\theta - \lambda_1 \left( 2\frac{k(\theta)}{\theta}\nabla\theta + \frac{\mathbf{q}}{\theta} \right). \tag{2.2.6}$$

Multiplying 2.2.5 by $\mathbf{D}$ and 2.2.6 by $\nabla\theta$ and summing results in

$$0 = 2\hat{\xi} - \lambda_1(2\hat{\xi} - \xi),$$

which means (using the constraint)

$$\lambda_1 = 2.$$

Taking trace of 2.2.5 leads to

$$\operatorname{tr}\mathbf{T} = -\frac{\lambda_2}{\lambda_1}d,$$

Let us now denote

$$p_m = -\frac{\lambda_2}{\lambda_1} = \frac{1}{d}\operatorname{tr}\mathbf{T}$$

as *mean normal stress*. This quantity $p$ does not have the meaning of thermodynamic pressure. It is just another unknown to be computed. Finally, we obtain well known Navier-Stokes-Fourier constitutive relations

$$\mathbf{T} = -p_m\mathbf{I} + 2\mu(\theta)\mathbf{D}, \tag{2.2.7}$$

$$\mathbf{q} = -k(\theta)\nabla\theta. \tag{2.2.8}$$

[7] Maximizing is performed only with respect to $\mathbf{D}$ and $\nabla\theta$. Other quantities as $\theta$ or $\rho$ are thought to be constant during the procedure.

### 2.2.4 Derivation of Incompressible Viscoelastic Models

In this subsection, we derive generalizations of several classical viscoelastic models with temperature dependent material coefficients. We are interested only in incompressible cases ($\operatorname{div}\mathbf{v}=0$) and we proceed in a very similar way as in [15]. For all further derived models we assume the elastic part of material response can be modelled as the response of Neo-Hookean solid. Hence we can prepare some identities resulting from this choice.

**Compressible case** For a compressible Neo-Hookean solid the free energy has the form

$$\hat{\psi}\left(\rho,\theta,\operatorname{tr}\mathbf{B}_{\kappa_p(t)},\det\mathbf{B}_{\kappa_p(t)}\right)=\hat{\psi}_0(\rho,\theta)+\frac{G(\theta)}{2\rho}\left(\operatorname{tr}\mathbf{B}_{\kappa_p(t)}-d-\ln\left(\det\mathbf{B}_{\kappa_p(t)}\right)\right). \tag{2.2.9}$$

with $G(\theta)$ denoting temperature dependent Young's modulus. The corresponding entropy balance (substituting $\hat{\psi}$ to 2.1.12 and using 2.2.3 and 2.2.4) reads

$$\begin{aligned}\rho\dot{\eta}&=-\operatorname{div}\frac{\mathbf{q}}{\theta}\\&\quad+\frac{1}{\theta}\left[(\mathbf{T}-G(\theta)(\mathbf{B}_{\kappa_p(t)}-\mathbf{I})):\mathbf{D}+G(\theta)(\mathbf{C}_{\kappa_p(t)}-\mathbf{I}):\mathbf{D}_{\kappa_p(t)}-\frac{\mathbf{q}\cdot\nabla\theta}{\theta}\right]+\rho\frac{r}{\theta}\end{aligned}$$

and therefore we have identified entropy production as follows

$$\xi=\left(\mathbf{T}-G(\theta)(\mathbf{B}_{\kappa_p(t)}-\mathbf{I})\right):\mathbf{D}+G(\theta)\left(\mathbf{C}_{\kappa_p(t)}-\mathbf{I}\right):\mathbf{D}_{\kappa_p(t)}-\frac{\mathbf{q}\cdot\nabla\theta}{\theta}. \tag{2.2.10}$$

Temperature evolution equation corresponding to the choice of $\hat{\psi}$ is

$$\begin{aligned}\rho c_v\dot{\theta}&=\left(\mathbf{T}-\left(G(\theta)-\theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)(\mathbf{B}_{\kappa_p(t)}-\mathbf{I})\right):\mathbf{D}\\&\quad+\left(G(\theta)-\theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)(\mathbf{C}_{\kappa_p(t)}-\mathbf{I}):\mathbf{D}_{\kappa_p(t)}-\operatorname{div}\mathbf{q}+\rho r.\end{aligned} \tag{2.2.11}$$

**Incompressible case** In the incompressible case, it seems very similar. The free energy has the form

$$\hat{\psi}\left(\rho,\theta,\operatorname{tr}\mathbf{B}_{\kappa_p(t)}\right)=\hat{\psi}_0(\rho,\theta)+\frac{G(\theta)}{2\rho}\left(\operatorname{tr}\mathbf{B}_{\kappa_p(t)}-d\right) \tag{2.2.12}$$

Analogously as in the compressible case, it can be shown (using 2.2.3) that this choice of $\hat{\psi}$ implies the entropy balance in the form

$$\rho\dot{\eta}=-\operatorname{div}\frac{\mathbf{q}}{\theta}+\frac{1}{\theta}\left[(\mathbf{T}-G(\theta)\mathbf{B}_{\kappa_p(t)}):\mathbf{D}+G(\theta)\mathbf{C}_{\kappa_p(t)}:\mathbf{D}_{\kappa_p(t)}-\frac{\mathbf{q}\cdot\nabla\theta}{\theta}\right]+\rho\frac{r}{\theta}.$$

Hence we identify the production of entropy as

$$\xi=(\mathbf{T}-G(\theta)\mathbf{B}_{\kappa_p(t)}):\mathbf{D}+G(\theta)\mathbf{C}_{\kappa_p(t)}:\mathbf{D}_{\kappa_p(t)}-\frac{\mathbf{q}\cdot\nabla\theta}{\theta}. \tag{2.2.13}$$

For this choice of $\hat{\psi}$, the evolution equation for temperature reads

$$\rho c_v \dot{\theta} = \left( \mathbf{T} - \left( G(\theta) - \theta \frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta} \right) \mathbf{B}_{\kappa_p(t)} \right) : \mathbf{D} + \left( G(\theta) - \theta \frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta} \right) \mathbf{C}_{\kappa_p(t)} : \mathbf{D}_{\kappa_p(t)} - \operatorname{div} \mathbf{q} + \rho r. \tag{2.2.14}$$

**T-Oldroyd-B Model**

The standard viscoelastic model Oldroyd-B can be expressed as

$$\mathbf{T} = -p\mathbf{I} + 2\mu_2 \mathbf{D} + G(\mathbf{B}_{\kappa_p(t)} - \mathbf{I}), \tag{2.2.15}$$

$$\overset{\triangledown}{\mathbf{B}}_{\kappa_p(t)} = -\frac{G}{\mu_1}(\mathbf{B}_{\kappa_p(t)} - \mathbf{I}), \tag{2.2.16}$$

where $p$ is additional unknown and material parameters are $G \geq 0$ Young's modulus, $\mu_1 \geq 0$ and $\mu_2 \geq 0$ viscosities.

Our goal is to derive the same model but with temperature dependent material parameters and appropriate temperature evolution equation. In order to do so, we consider incompressible case (ICC) and the elastic part of deformation behaving like a compressible Neo-Hookean solid. Hence an evolution equation for the temperature is 2.2.11 and an entropy production are expressed as 2.2.10

$$\xi = (\mathbf{T} - G(\theta)(\mathbf{B}_{\kappa_p(t)} - \mathbf{I})) : \mathbf{D} + G(\theta)(\mathbf{C}_{\kappa_p(t)} - \mathbf{I}) : \mathbf{D}_{\kappa_p(t)} - \frac{\mathbf{q} \cdot \nabla\theta}{\theta}.$$

Further, we prescribe the rate of entropy production as

$$\hat{\xi}(\mathbf{D}, \mathbf{D}_{\kappa_p(t)}, \nabla\theta) = 2\mu_2(\theta)\mathbf{D} : \mathbf{D} + 2\mu_1(\theta)\mathbf{D}_{\kappa_p(t)}\mathbf{C}_{\kappa_p(t)} : \mathbf{D}_{\kappa_p(t)} + \frac{k(\theta)}{\theta}\nabla\theta \cdot \nabla\theta,$$

where $k(\theta) \geq 0$ is heat conductivity. The second term is non-negative

$$\mathbf{D}_{\kappa_p(t)}\mathbf{C}_{\kappa_p(t)} : \mathbf{D}_{\kappa_p(t)} = \mathbf{F}_{\kappa_p(t)}\mathbf{D}_{\kappa_p(t)} : \mathbf{F}_{\kappa_p(t)}\mathbf{D}_{\kappa_p(t)} \geq 0,$$

thus for non-negative material coefficients it holds $\hat{\xi} \geq 0$ and the second law of thermodynamic is satisfied.

Next step is to maximize $\hat{\xi}(\mathbf{D}, \mathbf{D}_{\kappa_p(t)}, \nabla\theta)$ with respect to all three variables and considering a constraint $\hat{\xi} = \xi$. As we are dealing with the case (ICC) (see subsection 2.2.2), we should add only one constraint due to the incompressibility of the total deformation

$$\operatorname{div} \mathbf{v} = \operatorname{tr} \mathbf{D} = 0.$$

After defining Lagrange function

$$L(\mathbf{D}, \mathbf{D}_{\kappa_p(t)}, \nabla\theta) = \hat{\xi}(\mathbf{D}, \mathbf{D}_{\kappa_p(t)}, \nabla\theta) - \lambda_1(\hat{\xi}(\mathbf{D}, \mathbf{D}_{\kappa_p(t)}, \nabla\theta) - \xi) - \lambda_2(\operatorname{tr} \mathbf{D}),$$

necessary conditions for an extreme are

$$0 = \frac{\partial L}{\partial \mathbf{D}} = 4\mu_2(\theta)\mathbf{D} - \lambda_1 \left(4\mu_2(\theta)\mathbf{D} - \mathbf{T} + G(\theta)(\mathbf{B}_{\kappa_p(t)} - \mathbf{I})\right) - \lambda_2 \mathbf{I}, \tag{2.2.17}$$

$$0 = \frac{\partial L}{\partial \mathbf{D}_{\kappa_p(t)}} = 4\mu_1(\theta)\mathbf{D}_{\kappa_p(t)}\mathbf{C}_{\kappa_p(t)} - \lambda_1 \left(4\mu_1(\theta)\mathbf{D}_{\kappa_p(t)}\mathbf{C}_{\kappa_p(t)} - G(\theta)(\mathbf{C}_{\kappa_p(t)} - \mathbf{I})\right), \tag{2.2.18}$$

$$0 = \frac{\partial L}{\partial \nabla\theta} = 2\frac{k(\theta)}{\theta}\nabla\theta - \lambda_1 \left(2\frac{k(\theta)}{\theta}\nabla\theta + \frac{\mathbf{q}}{\theta}\right). \tag{2.2.19}$$

Considering 2.2.17 $\cdot\mathbf{D}$ + 2.2.18 $\cdot\mathbf{D}_{\kappa_p(t)}$ + 2.2.19 $\cdot\nabla\theta$ leads to

$$0 = 2\hat{\xi} - \lambda_1(2\hat{\xi} - \xi),$$

which means (using the constraint)

$$\lambda_1 = 2. \tag{2.2.20}$$

Taking trace of 2.2.17 gives

$$\frac{\lambda_2}{\lambda_1} d = -\mathrm{tr}\,\mathbf{T} + G(\theta)(\mathrm{tr}\mathbf{B}_{\kappa_p(t)} - d),$$

Let us now denote

$$p = \frac{\lambda_2}{\lambda_1}. \tag{2.2.21}$$

This quantity has neither the meaning of thermodynamic pressure nor the meaning of mean normal stress. It is just another unknown to be computed. From 2.2.17, 2.2.19, 2.2.20 and 2.2.21 we can get constitutive relations

$$\mathbf{T} = -p\mathbf{I} + 2\mu_2(\theta)\mathbf{D} + G(\theta)(\mathbf{B}_{\kappa_p(t)} - \mathbf{I}), \tag{2.2.22}$$

$$\mathbf{q} = -k(\theta)\nabla\theta. \tag{2.2.23}$$

But we need an evolution equation for the quantity $\mathbf{B}_{\kappa_p(t)}$. The second necessary condition can be now rewritten as

$$2\mu_1\mathbf{D}_{\kappa_p(t)}\mathbf{C}_{\kappa_p(t)} = G(\theta)(\mathbf{C}_{\kappa_p(t)} - \mathbf{I}). \tag{2.2.24}$$

If we consider $\mathbf{F}_{\kappa_p(t)}\cdot$ 2.2.24 $\cdot\mathbf{F}^{-1}_{\kappa_p(t)}$, we obtain

$$2\mu_1\mathbf{F}_{\kappa_p(t)}\mathbf{D}_{\kappa_p(t)}\mathbf{F}^{T}_{\kappa_p(t)} = G(\theta)(\mathbf{B}_{\kappa_p(t)} - \mathbf{I}),$$

which using 2.2.2 leads directly to

$$\overset{\triangledown}{\mathbf{B}}_{\kappa_p(t)} = -\frac{G(\theta)}{\mu_1(\theta)}(\mathbf{B}_{\kappa_p(t)} - \mathbf{I}). \tag{2.2.25}$$

The last step in derivation is rewriting temperature evolution equation 2.2.11 to a suitable form. The first term

$$(\mathbf{T} - \left(G(\theta) - \theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)(\mathbf{B}_{\kappa_p(t)} - \mathbf{I})) : \mathbf{D}$$

reduces to

$$2\mu_2(\theta)\mathbf{D}:\mathbf{D}+\theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\mathbf{B}_{\kappa_p(t)}:\mathbf{D}$$

due to the incompressibility condition $\operatorname{tr}\mathbf{D}=0$. The second term needs a bit more work. Using 2.2.24 and 2.2.25, we have

$$\begin{aligned}
G(\theta)(\mathbf{C}_{\kappa_p(t)}-\mathbf{I}):\mathbf{D}_{\kappa_p(t)} &= 2\mu_1(\theta)\mathbf{D}_{\kappa_p(t)}\mathbf{C}_{\kappa_p(t)}:\mathbf{D}_{\kappa_p(t)}\\
&= 2\mu_1(\theta)\mathrm{tr}\left(\mathbf{D}_{\kappa_p(t)}\mathbf{F}^T_{\kappa_p(t)}\mathbf{F}_{\kappa_p(t)}\mathbf{D}_{\kappa_p(t)}\right)\\
&= 2\mu_1(\theta)\mathrm{tr}\left(\mathbf{F}_{\kappa_p(t)}\mathbf{D}_{\kappa_p(t)}\mathbf{D}_{\kappa_p(t)}\mathbf{F}^T_{\kappa_p(t)}\right)\\
&= 2\mu_1(\theta)\mathrm{tr}\left(\mathbf{F}_{\kappa_p(t)}\mathbf{D}_{\kappa_p(t)}\mathbf{F}^T_{\kappa_p(t)}\mathbf{F}^{-T}_{\kappa_p(t)}\mathbf{F}^{-1}_{\kappa_p(t)}\mathbf{F}_{\kappa_p(t)}\mathbf{D}_{\kappa_p(t)}\mathbf{F}^T_{\kappa_p(t)}\right)\\
&= 2\mu_1(\theta)\mathrm{tr}\left(\overset{\triangledown}{\mathbf{B}}_{\kappa_p(t)}\,\mathbf{B}^{-1}_{\kappa_p(t)}\,\overset{\triangledown}{\mathbf{B}}_{\kappa_p(t)}\right). \qquad (2.2.26)
\end{aligned}$$

We can obtain yet another expression using 2.2.25

$$\begin{aligned}
2\mu_1(\theta)\mathrm{tr}\left(\overset{\triangledown}{\mathbf{B}}_{\kappa_p(t)}\,\mathbf{B}^{-1}_{\kappa_p(t)}\,\overset{\triangledown}{\mathbf{B}}_{\kappa_p(t)}\right) &= \frac{G^2(\theta)}{2\mu_1(\theta)}\mathrm{tr}\left((\mathbf{B}_{\kappa_p(t)}-\mathbf{I})\mathbf{B}^{-1}_{\kappa_p(t)}(\mathbf{B}_{\kappa_p(t)}-\mathbf{I})\right)\\
&= \frac{G^2(\theta)}{2\mu_1(\theta)}\mathrm{tr}\left(\mathbf{B}_{\kappa_p(t)}+\mathbf{B}^{-1}_{\kappa_p(t)}-2\mathbf{I}\right)\\
&= \frac{G^2(\theta)}{2\mu_1(\theta)}\left(\operatorname{tr}\mathbf{B}_{\kappa_p(t)}+\operatorname{tr}\mathbf{B}^{-1}_{\kappa_p(t)}-2d\right). \qquad (2.2.27)
\end{aligned}$$

Finally we can express the second term in 2.2.11 as

$$\begin{aligned}
\left(G(\theta)-\theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)(\mathbf{C}_{\kappa_p(t)}-\mathbf{I}):\mathbf{D}_{\kappa_p(t)} &= \left(1-\frac{\theta}{G(\theta)}\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)G(\theta)(\mathbf{C}_{\kappa_p(t)}-\mathbf{I}):\mathbf{D}_{\kappa_p(t)}\\
&= \left(1-\frac{\theta}{G(\theta)}\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)\frac{G^2(\theta)}{2\mu_1(\theta)}\left(\operatorname{tr}\mathbf{B}_{\kappa_p(t)}+\operatorname{tr}\mathbf{B}^{-1}_{\kappa_p(t)}-2d\right)\\
&= \left(G(\theta)-\theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)\frac{G(\theta)}{2\mu_1(\theta)}\left(\operatorname{tr}\mathbf{B}_{\kappa_p(t)}+\operatorname{tr}\mathbf{B}^{-1}_{\kappa_p(t)}-2d\right). \qquad (2.2.28)
\end{aligned}$$

The third term in 2.2.11 reads

$$-\operatorname{div}\mathbf{q}=\operatorname{div}\left(k(\theta)\nabla\theta\right) \qquad (2.2.29)$$

We have derived the complete model with temperature dependent coefficients and temperature evolution equation

$$\mathbf{T} = -p\mathbf{I} + 2\mu_2(\theta)\mathbf{D} + G(\theta)(\mathbf{B}_{\kappa_p(t)} - \mathbf{I}), \tag{2.2.30}$$

$$\mathbf{q} = -k(\theta)\nabla\theta, \tag{2.2.31}$$

$$\overset{\triangledown}{\mathbf{B}}_{\kappa_p(t)} = -\frac{G(\theta)}{\mu_1(\theta)}(\mathbf{B}_{\kappa_p(t)} - \mathbf{I}), \tag{2.2.32}$$

$$\begin{aligned}\rho c_v\dot{\theta} = {} & 2\mu_2(\theta)\mathbf{D} : \mathbf{D} + \theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\mathbf{B}_{\kappa_p(t)} : \mathbf{D} \\ & + \left(G(\theta) - \theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)\frac{G(\theta)}{2\mu_1(\theta)}\left(\operatorname{tr}\mathbf{B}_{\kappa_p(t)} + \operatorname{tr}\mathbf{B}^{-1}_{\kappa_p(t)} - 2d\right) + \operatorname{div}\left(k(\theta)\nabla\theta\right) + \rho r.\end{aligned} \tag{2.2.33}$$

Let us call it T-Oldroyd-B.

### T-Maxwell Model

Standard Maxwell model can be written as

$$\mathbf{T} = -p\mathbf{I} + G(\mathbf{B}_{\kappa_p(t)} - \mathbf{I}), \tag{2.2.34}$$

$$\overset{\triangledown}{\mathbf{B}}_{\kappa_p(t)} = -\frac{G}{\mu_1}(\mathbf{B}_{\kappa_p(t)} - \mathbf{I}), \tag{2.2.35}$$

where $p$ is additional unknown and material parameters are $G \geq 0$ Young's modulus and $\mu \geq 0$ viscosity.

The Maxwell model is a special case of the Oldroyd-B model with $\mu_2 = 0$. Hence derivation of the same model with temperature dependent coefficients is analogous to the previous derivation of the model T-Oldroyd-B with the only one difference: the rate of entropy production is considered as

$$\hat{\xi}(\mathbf{D}_{\kappa_p(t)}, \nabla\theta) = 2\mu_1(\theta)\mathbf{D}_{\kappa_p(t)}\mathbf{C}_{\kappa_p(t)} : \mathbf{D}_{\kappa_p(t)} + \frac{k(\theta)}{\theta}\nabla\theta \cdot \nabla\theta.$$

All other steps in the derivation are analogous as before and we obtain

$$\mathbf{T} = -p\mathbf{I} + G(\theta)(\mathbf{B}_{\kappa_p(t)} - \mathbf{I}), \tag{2.2.36}$$

$$\mathbf{q} = -k(\theta)\nabla\theta, \tag{2.2.37}$$

$$\overset{\triangledown}{\mathbf{B}}_{\kappa_p(t)} = -\frac{G(\theta)}{\mu_1(\theta)}(\mathbf{B}_{\kappa_p(t)} - \mathbf{I}), \tag{2.2.38}$$

$$\begin{aligned}\rho c_v\dot{\theta} = {} & \theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\mathbf{B}_{\kappa_p(t)} : \mathbf{D} + \left(G(\theta) - \theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)\frac{G(\theta)}{2\mu_1(\theta)}\left(\operatorname{tr}\mathbf{B}_{\kappa_p(t)} + \operatorname{tr}\mathbf{B}^{-1}_{\kappa_p(t)} - 2d\right) \\ & + \operatorname{div}\left(k(\theta)\nabla\theta\right) + \rho r.\end{aligned} \tag{2.2.39}$$

We call this model T-Maxwell. Note that the model is very similar to the T-Maxwell model derived from mechanical analogues in the section.

### T-Quad1 Model

Model Quad1 is a model with purely quadratic rate of entropy production (or dissipation). It was proposed in [15] and reads [8]

$$\mathbf{T} = -p\mathbf{I} + 2\mu_2\mathbf{D} + G\mathbf{B}^d_{\kappa_p(t)}, \tag{2.2.40}$$

$$\overset{\triangledown}{\mathbf{B}}_{\kappa_p(t)} = -\frac{G(\theta)}{\mu_1(\theta)}\mathbf{B}_{\kappa_p(t)}\mathbf{B}^d_{\kappa_p(t)}, \tag{2.2.41}$$

where $p$ is additional unknown meaning mean normal stress and material parameters are $G \geq 0$ Young's modulus, $\mu_1 \geq 0$ and $\mu_2 \geq 0$ viscosities. The parameters are the same as for Oldroyd-B. In fact, this model is a generalization of Oldroyd-B model because Oldroyd-B can be obtained by linearization of Quad1, which is shown in [15]. The model Quad1 was derived in [15] using the thermodynamic framework proposed here, specially for the incompressible case (III) with Neo-Hookean free energy 2.2.12

$$\hat{\psi} = \hat{\psi}_0(\rho,\theta) + \frac{G}{2\rho}\left(\operatorname{tr}\mathbf{B}_{\kappa_p(t)} - d\right)$$

and quadratic rate of entropy production

$$\hat{\xi}(\mathbf{D},\mathbf{D}_{\kappa_p(t)}) = 2\mu_2\mathbf{D}:\mathbf{D} + 2\mu_1\mathbf{D}_{\kappa_p(t)}:\mathbf{D}_{\kappa_p(t)}.$$

We follow the derivation and add temperature dependence to material coefficients and temperature gradient to the rate of entropy production. Thus we start with

$$\hat{\psi} = \hat{\psi}_0(\rho,\theta) + \frac{G(\theta)}{2\rho}\left(\operatorname{tr}\mathbf{B}_{\kappa_p(t)} - d\right),$$

$$\hat{\xi}(\mathbf{D},\mathbf{D}_{\kappa_p(t)}) = 2\mu_2(\theta)\mathbf{D}:\mathbf{D} + 2\mu_1(\theta)\mathbf{D}_{\kappa_p(t)}:\mathbf{D}_{\kappa_p(t)} + \frac{k(\theta)}{\theta}\nabla\theta:\nabla\theta,$$

where material parameters are Young's modulus $G(\theta) \geq 0$, viscosities $\mu_1(\theta) \geq 0$, $\mu_2(\theta) \geq 0$ and heat conductivity $k(\theta) \geq 0$. Since elastic response is supposed to be incompressible Neo-Hookean, we can identify entropy production $\xi$ as 2.2.13

$$\xi = (\mathbf{T} - G(\theta)\mathbf{B}_{\kappa_p(t)}):\mathbf{D} + G(\theta)\mathbf{C}_{\kappa_p(t)}:\mathbf{D}_{\kappa_p(t)} - \frac{\mathbf{q}\cdot\nabla\theta}{\theta}.$$

Now we maximize the function $\hat{\xi}(\mathbf{D},\mathbf{D}_{\kappa_p(t)},\nabla\theta)$ with respect to all three variables. Except of omnipresent constraint $\hat{\xi} = \xi$, we also have to consider constraints

$$\operatorname{tr}\mathbf{D} = 0 \qquad \text{and} \qquad \operatorname{tr}\mathbf{D}_{\kappa_p(t)} = 0$$

[8] Notation

$$\mathbf{A}^d = \mathbf{A} - \frac{1}{3}\operatorname{tr}\mathbf{A}\mathbf{I}$$

means *the deviatoric part of a tensor* $\boldsymbol{A}$ (or also called *the traceless part*).

due to the case (III) (see 2.2.2). After defining Lagrange function

$$L(\mathbf{D}, \mathbf{D}_{\kappa_p(t)}, \nabla\theta) = \hat{\xi}(\mathbf{D}, \mathbf{D}_{\kappa_p(t)}, \nabla\theta) \\ - \lambda_1(\hat{\xi}(\mathbf{D}, \mathbf{D}_{\kappa_p(t)}, \nabla\theta) - \xi) - \lambda_2(\operatorname{tr}\mathbf{D}) + \lambda_3(\operatorname{tr}\mathbf{D}_{\kappa_p(t)}),$$

necessary conditions for an extreme are

$$0 = \frac{\partial L}{\partial \mathbf{D}} = 4\mu_2(\theta)\mathbf{D} - \lambda_1\left(4\mu_2(\theta)\mathbf{D} - \mathbf{T} + G(\theta)\mathbf{B}_{\kappa_p(t)}\right) - \lambda_2\mathbf{I}, \tag{2.2.42}$$

$$0 = \frac{\partial L}{\partial \mathbf{D}_{\kappa_p(t)}} = 4\mu_1(\theta)\mathbf{D}_{\kappa_p(t)} - \lambda_1\left(4\mu_1(\theta)\mathbf{D}_{\kappa_p(t)} - G(\theta)\mathbf{C}_{\kappa_p(t)}\right) - \lambda_3\mathbf{I}, \tag{2.2.43}$$

$$0 = \frac{\partial L}{\partial \nabla\theta} = 2\frac{k(\theta)}{\theta}\nabla\theta - \lambda_1\left(2\frac{k(\theta)}{\theta}\nabla\theta + \frac{\mathbf{q}}{\theta}\right). \tag{2.2.44}$$

Considering 2.2.42 $\cdot\mathbf{D}$ + 2.2.43 $\cdot\mathbf{D}_{\kappa_p(t)}$ + 2.2.44 $\cdot\nabla\theta$ leads to

$$0 = 2\hat{\xi} - \lambda_1(2\hat{\xi} - \xi),$$

which means (using the constraint)

$$\lambda_1 = 2. \tag{2.2.45}$$

Taking trace of 2.2.42 gives

$$d\frac{\lambda_2}{\lambda_1} = -\operatorname{tr}(\mathbf{T} + G(\theta)\mathbf{B}_{\kappa_p(t)}), \tag{2.2.46}$$

Let us now denote

$$p = \frac{1}{d}\operatorname{tr}\mathbf{T} \tag{2.2.47}$$

*mean normal stress*. Considering 2.2.45, we get constitutive relation for $\mathbf{T}$ from 2.2.42 using 2.2.46, 2.2.47 and constitutive relation for $\mathbf{q}$ from 2.2.44

$$\mathbf{T} = -p\mathbf{I} + 2\mu_2(\theta)\mathbf{D} + G(\theta)\mathbf{B}^d_{\kappa_p(t)}, \tag{2.2.48}$$

$$\mathbf{q} = -k(\theta)\nabla\theta. \tag{2.2.49}$$

We need en evolution equation for the quantity $\mathbf{B}_{\kappa_p(t)}$. Substituting 2.2.45 into 2.2.43 leads to

$$2\mu_1\mathbf{D}_{\kappa_p(t)} = G(\theta)\mathbf{C}_{\kappa_p(t)} + \frac{\lambda_3}{\lambda_1}\mathbf{I}. \tag{2.2.50}$$

By taking trace of 2.2.43 we conclude that

$$\frac{\lambda_3}{\lambda_1} = -\frac{G(\theta)}{d}\operatorname{tr}\mathbf{C}_{\kappa_p(t)}. \tag{2.2.51}$$

If we consider $\mathbf{F}_{\kappa_p(t)}\cdot$ 2.2.50 $\cdot\mathbf{F}^T_{\kappa_p(t)}$ and substitute 2.2.51, we obtain

$$2\mu_1\mathbf{F}_{\kappa_p(t)}\mathbf{D}_{\kappa_p(t)}\mathbf{F}^T_{\kappa_p(t)} = G(\theta)\mathbf{B}_{\kappa_p(t)}\left(\mathbf{B}_{\kappa_p(t)} - \frac{1}{3}(\operatorname{tr}\mathbf{B}_{\kappa_p(t)})\mathbf{I}\right),$$

which using 2.2.2 leads directly to

$$\overset{\triangledown}{\mathbf{B}}_{\kappa_p(t)} = -\frac{G(\theta)}{\mu_1(\theta)}\mathbf{B}_{\kappa_p(t)}\mathbf{B}^d_{\kappa_p(t)}. \tag{2.2.52}$$

The last step in derivation is rewriting temperature evolution equation 2.2.14 to a suitable form. The first term

$$(\mathbf{T} - \left(G(\theta) - \theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)\mathbf{B}_{\kappa_p(t)} : \mathbf{D}$$

reduces to

$$2\mu_2(\theta)\mathbf{D} : \mathbf{D} + \theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\mathbf{B}_{\kappa_p(t)} : \mathbf{D}$$

due to the incompressibility condition $\operatorname{tr}\mathbf{D} = 0$. Using 2.2.2 and 2.2.52, we rewrite the second term as

$$\begin{aligned}\left(G(\theta) - \theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)\mathbf{C}_{\kappa_p(t)} : \mathbf{D}_{\kappa_p(t)} &= \left(G(\theta) - \theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)\operatorname{tr}\left(\mathbf{F}_{\kappa_p(t)}\mathbf{D}_{\kappa_p(t)}\mathbf{F}^T_{\kappa_p(t)}\right)\\ &= -\left(G(\theta) - \theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)\operatorname{tr}\ \overset{\triangledown}{\mathbf{B}}_{\kappa_p(t)}\\ &= \left(G(\theta) - \theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)\frac{G(\theta)}{2\mu_1(\theta)}\operatorname{tr}\left(\mathbf{B}_{\kappa_p(t)}\mathbf{B}^d_{\kappa_p(t)}\right)\\ &= \left(G(\theta) - \theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)\frac{G(\theta)}{2\mu_1(\theta)}\mathbf{B}^d_{\kappa_p(t)} : \mathbf{B}^d_{\kappa_p(t)}.\end{aligned} \tag{2.2.53}$$

The third term in 2.2.11 reads

$$-\operatorname{div}\mathbf{q} = \operatorname{div}\left(k(\theta)\nabla\theta\right) \tag{2.2.54}$$

We have derived the complete model with temperature dependent coefficients and also with the evolution equation for temperature presented the previous chapter.

$$\mathbf{T} = -p\mathbf{I} + 2\mu_2(\theta)\mathbf{D} + G(\theta)\mathbf{B}^d_{\kappa_p(t)}, \tag{2.2.55}$$

$$\mathbf{q} = -k(\theta)\nabla\theta, \tag{2.2.56}$$

$$\overset{\triangledown}{\mathbf{B}}_{\kappa_p(t)} = -\frac{G(\theta)}{\mu_1(\theta)}\mathbf{B}_{\kappa_p(t)}\mathbf{B}^d_{\kappa_p(t)}, \tag{2.2.57}$$

$$\begin{aligned}\rho c_v\dot{\theta} &= 2\mu_2(\theta)\mathbf{D} : \mathbf{D} + \theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\mathbf{B}_{\kappa_p(t)} : \mathbf{D}\\ &\quad + \left(G(\theta) - \theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)\frac{G(\theta)}{2\mu_1(\theta)}\mathbf{B}^d_{\kappa_p(t)} : \mathbf{B}^d_{\kappa_p(t)} + \operatorname{div}\left(k(\theta)\nabla\theta\right) + \rho r.\end{aligned} \tag{2.2.58}$$

We call this model T-Quad1.

# 3. Simulations in 2D

For simplicity's sake we denote $\mathbf{B}$ as an abbreviation of $\mathbf{B}_{\kappa_p(t)}$ and define $\mathbf{D}(v) = \Big((\nabla \mathbf{v}) + (\nabla \mathbf{v})^T\Big)$ in this chapter.

## 3.1 Weak Formulation of Derived Models

If we want to use the Finite element method, we have to convert the problem into a weak formulation with initial and boundary conditions for the initial and boundary value problem. We have to determine an appropriate space, to which the weak solution belongs. In order to do so, a consideration about a priori estimates for sought quantities is carried out.

### 3.1.1 Initial and Boundary Conditions

We suppose the material is relaxed in time $t = 0$, therefore

$$\begin{aligned} \mathbf{v}(t=0) &= 0, \\ \mathbf{p}(t=0) &= 0, \\ \mathbf{B}(t=0) &= \mathbf{I} \end{aligned}$$

and the initial state of the temperature is

$$\theta(t=0) = \theta_0.$$

Further, we split the boundary $\partial\Omega$ of the computation domain $\Omega$ into two disjoint parts $\Gamma_D$ and $\Gamma_N$ so that $\overline{\Gamma_D \cup \Gamma_N} = \partial\Omega$. In a standard way, we prescribe Dirichlet boundary condition and the traction

$$\begin{aligned} \mathbf{v}(t) &= v_D(t), \text{ on } \Gamma_D, \\ \mathbf{Tn}(t) &= \mathbf{t}(t), \text{ on } \Gamma_N, \end{aligned}$$

respectively. Let us split the boundary of $\Omega$ once again into two disjoint parts $\Theta_D$ and $\Theta_N$ so that $\overline{\Theta_D \cup \Theta_N} = \partial\Omega$ in order to define the heat flux and Dirichlet boundary condition for temperature as

$$\begin{aligned} \mathbf{q}(t) \cdot \mathbf{n} &= q_N(t), \text{ on } \Omega_N, \\ \theta(t) &= \theta_D(t), \text{ on } \Omega_D, \end{aligned}$$

respectively. We do not prescribe any boundary conditions for $\mathbf{B}$.

### 3.1.2 A Priori Estimates

A priori estimates (except for the estimate for the temperature) for our models can be adopted from [15]. We add only non-negative temperature dependent material coefficients: Young's modulus $G(\theta) \geq 0$ and viscosity $\mu(\theta) \geq 0$. We suppose they belong to the space $L^\infty(0, T; L^\infty(\Omega))$ (this is not a restrictive assumption due

to their physical interpretation). Hence all estimates hold for all three models T-Maxwell, T-Oldroyd-B, T-Quad1.

$$||\mathbf{v}||_{L^{10/3}((0,T)\times\Omega)^d} \leq C, \quad ||\mathbf{B}||_{L^\infty(0,T;L^1(\Omega))^{d\times d}} \leq C, \quad ||p||_{L^{5/3}(0,T;L^1(\Omega))} \leq C.$$

We need the estimate for the temperature, but it seems like a very hard problem. An estimate for the Navier-Stokes-Fourier problem, which is close to our problem, is done in [3] and states that

$$\theta \in L^\infty(0,T;L^1(\Omega)) \tag{3.1.1}$$

$$\nabla\theta^{1/2-\lambda/2} \in L^2(0,T;L^2(\Omega)) \quad \text{for all small } \lambda > 0, \tag{3.1.2}$$

under the assumption, that $c_V\theta = e$, where $e$ is a specific internal energy. We do not have explicit constitutive relation between $\theta$ and $e$. We have only en evolution equation for $\theta$ with indefinite terms making estimation harder. This topic we leave for another research.

### 3.1.3 Weak Formulation for Initial and Boundary Value Problem

We can now define the weak formulation of our models. However, we search a solution in a bit different spaces than the suggested a priori estimates. For example we need to control the norm $||\nabla\theta(t)||$ hence we need to assume $\theta(t) \in W^{1,2}(\Omega)$. The chosen spaces are

$$\begin{aligned} V &:= L^2(0,T;W^{1,2}(\Omega))^d, \\ P &:= L^2(0,T;L^2(\Omega)), \\ B &:= L^2(0,T;W^{1,2}(\Omega))^{d\times d}, \\ \Theta &:= L^2(0,T;W^{1,2}(\Omega)), \end{aligned}$$

$$\begin{aligned} V_0 &:= L^2(0,T;W^{1,2}_{0,\Gamma_D}(\Omega))^d, \\ \Theta_0 &:= L^2(0,T;W^{1,2}_{0,\Theta_D}(\Omega)). \end{aligned}$$

#### T-Oldroyd-B

Let us define the weak solution of the model T-Oldroyd-B as follows: The quadruple $(\mathbf{v}, p, \mathbf{B}, \theta) \in V \times P \times B \times \Theta$, such that $\mathbf{v} - \tilde{\mathbf{v}} \in V_0$ and $\theta - \tilde{\theta} \in \Theta_0$, is the

weak solution of the model T-Oldroyd-B in $\Omega \subset \mathbb{R}^d$ if

$$\begin{aligned}
\int_\Omega \mathrm{tr}(\nabla \mathbf{v})\varphi \,\mathrm{dx} &= 0,\\
\int_\Omega \rho\left[\frac{\partial \mathbf{v}}{\partial t} + (\nabla \mathbf{v})\mathbf{v} - \mathbf{b}\right]\cdot \boldsymbol{\varphi}\,\mathrm{dx} + \int_\Omega \mathbf{T} : \nabla \boldsymbol{\varphi}\,\mathrm{dx} - \int_{\Gamma_N} \mathbf{t}\cdot\boldsymbol{\varphi}\,\mathrm{dS} &= 0,\\
\int_\Omega \left[\frac{\partial \mathbf{B}}{\partial t} + (\nabla \mathbf{B})\mathbf{v} - (\nabla \mathbf{v})\mathbf{B} - \mathbf{B}(\nabla \mathbf{v})^T + \frac{G(\theta)}{\mu_1(\theta)}(\mathbf{B}-\mathbf{I})\right] : \boldsymbol{\Phi}\,\mathrm{dx} &= 0,\\
\int_\Omega \Big[\rho\Big(c_V\frac{\partial \theta}{\partial t} + c_V(\nabla\theta)\cdot\mathbf{v} - r\Big) - \frac{\mu_2(\theta)}{2}\Big((\nabla\mathbf{v}) + (\nabla\mathbf{v})^T\Big) : \Big((\nabla\mathbf{v}) + (\nabla\mathbf{v})^T\Big)&\\
-\frac{\theta}{2}\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\mathbf{B} : \Big((\nabla\mathbf{v}) + (\nabla\mathbf{v})^T\Big)&\\
-\Big(G(\theta) - \theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\Big)\frac{G(\theta)}{2\mu_1(\theta)}\Big(\mathrm{tr}\mathbf{B} + \mathrm{tr}(\mathbf{B}^{-1}) - 2d\Big)\Big]\varphi_\theta\,\mathrm{dx}&\\
+\int_\Omega (k(\theta)\nabla\theta)\cdot\nabla\varphi_\theta\,\mathrm{dx} - \int_{\Theta_N} q_N\varphi_\theta\,\mathrm{dS} &= 0,\\
\text{where}\quad \mathbf{T} = -p\mathbf{I} + \mu_2(\theta)\Big((\nabla\mathbf{v}) + (\nabla\mathbf{v})^T\Big) + G(\theta)(\mathbf{B}-\mathbf{I})&
\end{aligned}$$

is satisfied for all $(\boldsymbol{\varphi}, \varphi, \boldsymbol{\Phi}, \varphi_\theta) \in V_0 \times P \times B \times \Theta_0$ and almost all $t \in (0,T)$, where $\tilde{\mathbf{v}}|_{\Gamma_D} = \mathbf{v}_D$, $\tilde{\theta}|_{\Theta_D} = \theta_D$ and $r \in L^2(0,T;L^2(\Omega))$, $\mathbf{b} \in L^2(0,T;L^2(\Omega))^d$.

**T-Quad1**

Let us define the weak solution of the model T-Quad1 as follows: The quadruple $(\mathbf{v}, p, \mathbf{B}, \theta) \in V \times P \times B \times \Theta$, such that $\mathbf{v} - \tilde{\mathbf{v}} \in V_0$ and $\theta - \tilde{\theta} \in \Theta_0$, is the weak solution of the model T-Quad1 in $\Omega \subset \mathbb{R}^d$ if

$$\begin{aligned}
\int_\Omega \mathrm{tr}(\nabla \mathbf{v})\varphi \,\mathrm{dx} &= 0,\\
\int_\Omega \rho\left[\frac{\partial \mathbf{v}}{\partial t} + (\nabla \mathbf{v})\mathbf{v} - \mathbf{b}\right]\cdot \boldsymbol{\varphi}\,\mathrm{dx} + \int_\Omega \mathbf{T} : \nabla \boldsymbol{\varphi}\,\mathrm{dx} - \int_{\Gamma_N} \mathbf{t}\cdot\boldsymbol{\varphi}\,\mathrm{dS} &= 0,\\
\int_\Omega \left[\frac{\partial \mathbf{B}}{\partial t} + (\nabla \mathbf{B})\mathbf{v} - (\nabla \mathbf{v})\mathbf{B} - \mathbf{B}(\nabla \mathbf{v})^T + \frac{G(\theta)}{\mu_1(\theta)}\mathbf{B}\mathbf{B}^d\right] : \boldsymbol{\Phi}\,\mathrm{dx} &= 0,\\
\int_\Omega \Big[\rho\Big(c_V\frac{\partial \theta}{\partial t} + c_V(\nabla\theta)\cdot\mathbf{v} - r\Big) - \frac{\mu_2(\theta)}{2}\mathbf{D}(v) : \mathbf{D}(v) - \frac{\theta}{2}\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\mathbf{B} : \mathbf{D}(v)&\\
-\Big(G(\theta) - \theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\Big)\frac{G(\theta)}{2\mu_1(\theta)}\Big(\mathbf{B} : \mathbf{B}^d\Big)\Big]\varphi_\theta\,\mathrm{dx} + \int_\Omega (k(\theta)\nabla\theta)\cdot\nabla\varphi_\theta\,\mathrm{dx} - \int_{\Theta_N} q_N\varphi_\theta\,\mathrm{dS} &= 0,\\
\text{where}\quad \mathbf{T} = -p\mathbf{I} + \mu_2(\theta)\mathbf{D}(v) + G(\theta)\mathbf{B}^d&
\end{aligned}$$

is satisfied for all $(\boldsymbol{\varphi}, \varphi, \boldsymbol{\Phi}, \varphi_\theta) \in V_0 \times P \times B \times \Theta_0$ and almost all $t \in (0,T)$, where $\tilde{\mathbf{v}}|_{\Gamma_D} = \mathbf{v}_D$, $\tilde{\theta}|_{\Theta_D} = \theta_D$ and $r \in L^2(0,T;L^2(\Omega))$, $\mathbf{b} \in L^2(0,T;L^2(\Omega))^d$.

## 3.2 Finite Element Method

A weakly formulated problem can be solved by the Finite element method (FEM), for more details see [2]. We have implemented this method with the aid of a free software FEniCS Project [10]. We have also used the open source software ParaView [1] to view the results and GMSH [7] to generate a computational mesh. The source codes can be found on the attached CD.

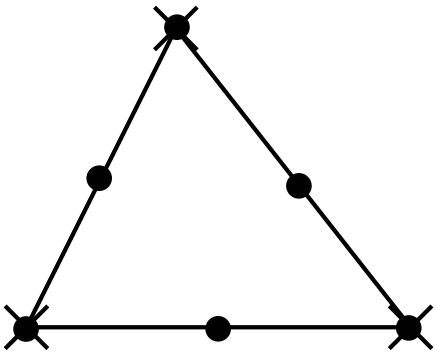


Figure 3.1: A typical element of triangulation with locations of the degrees of freedom. The crosses stand for $P_1$ elements, the dots for $P_2$ elements.

### 3.2.1 Discretization

In the previous section we introduced a weak formulation of the problem. The finite element method is based on the reformulation of an infinite-dimensional problem into a finite-dimensional one. The spaces where the solution is sought and the space of the test functions are replaced with their (finite-dimensional) approximations, also the domain $\Omega$ is replaced with its polygonal approximation $\Omega_h$ divided by triangulation. A typical element of the triangulation is depicted on (3.1).

Let us denote

- $\mathsf{P}_k(\Omega_h) := \{p \in C^0(\Omega_h) \mid \quad p|_T \in \mathcal{P}_k(T)\ ;\ T \text{ is an element of a triangulation of } \Omega_h\}$, where $\mathcal{P}_k(T)$ denotes a set of polynomials of the maximum degree $k \in \mathbb{N}$.

and then

- $V_h := \mathsf{P}_2^d(\Omega_h)$ as the space of piecewise quadratic $d$-dimensional vector functions on $\Omega_h$,
- $P_h := \mathsf{P}_1(\Omega_h)$ as the space of piecewise linear functions on $\Omega_h$,
- $B_h := \mathsf{P}_2^{d\times d}(\Omega_h)$ as the space of piecewise quadratic $d\times d$-dimensional tensor functions on $\Omega_h$,
- $\Theta_h := \mathsf{P}_2(\Omega_h)$ as the space of piecewise quadratic functions on $\Omega_h$,
- $V_{h0} := \{\psi \in V_h \mid \quad \psi|_{\Gamma_D} = 0\}$,
- $\Theta_{h0} := \{\psi \in \Theta_h \mid \quad \psi|_{\Theta_D} = 0\}$.

Time discretization is done using the $\Theta$-method, for example the Crank-Nicolson method for $\Theta = 0.5$ which is implicit and conditionally stable second order finite difference method. For $n \in \mathbb{N}$ and $\Delta t := T/n$ we split the interval $(0, T)$ into equidistant time steps $t_i := i\,\Delta t$, $i = 0, 1, 2, \ldots, n$ and denote $f^n := f(t_n)$ for any function $f(t)$. Now we can define the Galerkin system for each model for $\Theta \in [0, 1]$.

**T-Oldroyd**

Supposing there exist

$$\tilde{\mathbf{v}}_h \in V_h \text{ satisfying } \tilde{\mathbf{v}}_h|_{\Gamma_D} = \mathbf{v}_D,$$

$$\tilde{\theta}_h \in \Theta_h \text{ satisfying } \tilde{\theta}_h|_{\Theta_D} = \theta_D,$$

the problem is to find a quadruple $(\mathbf{v}_h, p_h, \mathbf{B}_h, \theta_h) \in V_h \times P_h \times B_h \times \Theta_h$ such that $\mathbf{v}_h - \tilde{\mathbf{v}}_h \in V_{h0}$, $\theta_h - \tilde{\theta} \in \Theta_{h0}$ and for all $(\boldsymbol{\varphi}_h, \varphi_h, \boldsymbol{\Phi}_h, \varphi_{\theta_h}) \in V_{h0} \times P_h \times B_h \times \Theta_{h0}$ and for $i = 1, 2, \ldots, n$ (considering initial conditions from 3.1.1) satisfying

$$\begin{aligned}
P^{n+1} &= 0,\\
\int_{\Omega_h} \rho \frac{\mathbf{v}_h^{n+1} - \mathbf{v}_h^n}{\Delta t} \cdot \boldsymbol{\varphi}_h \,\mathrm{dx} + \Theta V^{n+1} + (1-\Theta)V^n &= 0,\\
\int_{\Omega} \frac{\mathbf{B}_h^{n+1} - \mathbf{B}_h^n}{\Delta t} : \boldsymbol{\Phi}_{\boldsymbol{h}} \,\mathrm{dx} + \Theta B^{n+1} + (1-\Theta)B^n &= 0,\\
\int_{\Omega} \rho c_V \frac{\theta_h^{n+1} - \theta_h^n}{\Delta t} \varphi_{\theta h} \,\mathrm{dx} + \Theta T^{n+1} + (1-\Theta)T^n &= 0,
\end{aligned}$$

where we use

$$\begin{aligned}
P^n &:= \int_{\Omega_h} \mathrm{tr}(\nabla \mathbf{v}_h^n)\varphi_h \,\mathrm{dx},\\
V^n &:= \int_{\Omega_h} \rho\left[(\nabla \mathbf{v}_h^n)\mathbf{v}_h^n - \mathbf{b}^n\right] \cdot \boldsymbol{\varphi}_h \,\mathrm{dx} - \int_{\Omega_h} \mathbf{T}_h^n : \nabla \boldsymbol{\varphi}_h \,\mathrm{dx} + \int_{\Gamma_N} \mathbf{t}^n \cdot \boldsymbol{\varphi}_h \,\mathrm{dS},\\
&\quad \text{where } \mathbf{T}_h^n = -p_h^n \mathbf{I} + \mu_2(\theta_h^n)\left((\nabla \mathbf{v}_h^n) + (\nabla \mathbf{v}_h^n)^T\right) + G(\theta)\left(\mathbf{B}_h^n - \mathbf{I}\right),\\
B^n &:= \int_{\Omega} \left[(\nabla \mathbf{B}_h^n)\mathbf{v}_h^n - (\nabla \mathbf{v}_h^n)\mathbf{B}_h^n - \mathbf{B}_h^n(\nabla \mathbf{v}_h^n)^T + \frac{G(\theta_h^n)}{\mu_1(\theta_h^n)}(\mathbf{B}_h^n - \mathbf{I})\right] : \boldsymbol{\Phi}_{\boldsymbol{h}} \,\mathrm{dx},\\
T^n &:= \int_{\Omega} \Big[\rho\Big(c_V(\nabla \theta_h^n) \cdot \mathbf{v}_h^n - r^n\Big) - \frac{\mu_2(\theta_h^n)}{2}\left((\nabla \mathbf{v}_h^n) + (\nabla \mathbf{v}_h^n)^T\right) : \left((\nabla \mathbf{v}_h^n) + (\nabla \mathbf{v}_h^n)^T\right) +\\
&\quad \frac{G^2(\theta_h^n)}{2\mu_1(\theta_h^n)}\left(\mathrm{tr}\mathbf{B}_h^n + \mathrm{tr}(\mathbf{B}_h^n)^{-1} - 2d\right)\Big]\varphi_{\theta h} \,\mathrm{dx} + \int_{\Omega} (k(\theta_h^n)\nabla \theta_h^n) \cdot \nabla \varphi_{\theta h} \,\mathrm{dx} + \int_{\Theta_N} q_N^n \varphi_{\theta h} \,\mathrm{dS}.
\end{aligned}$$

**T-Quad1**

Supposing there exist

$$\tilde{\mathbf{v}}_h \in V_h \text{ satisfying } \tilde{\mathbf{v}}_h|_{\Gamma_D} = \mathbf{v}_D,$$

$$\tilde{\theta}_h \in \Theta_h \text{ satisfying } \tilde{\theta}_h|_{\Theta_D} = \theta_D,$$

the problem is to find a quadruple $(\mathbf{v}_h, p_h, \mathbf{B}_h, \theta_h) \in V_h \times P_h \times B_h \times \Theta_h$ such that $\mathbf{v}_h - \tilde{\mathbf{v}}_h \in V_{h0}$, $\theta_h - \tilde{\theta} \in \Theta_{h0}$ and for all $(\boldsymbol{\varphi}_h, \varphi_h, \boldsymbol{\Phi}_h, \varphi_{\theta_h}) \in V_{h0} \times P_h \times B_h \times \Theta_{h0}$ and for $i = 1, 2, \ldots, n$ (considering initial conditions from 3.1.1) satisfying

$$
\begin{aligned}
P^{n+1} &= 0,\\
\int_{\Omega_h} \rho \frac{\mathbf{v}_h^{n+1} - \mathbf{v}_h^n}{\Delta t} \cdot \boldsymbol{\varphi}_h \,\mathrm{dx} + \Theta V^{n+1} + (1-\Theta) V^n &= 0,\\
\int_{\Omega} \frac{\mathbf{B}_h^{n+1} - \mathbf{B}_h^n}{\Delta t} : \boldsymbol{\Phi}_{\boldsymbol{h}} \,\mathrm{dx} + \Theta B^{n+1} + (1-\Theta) B^n &= 0,\\
\int_{\Omega} \rho c_V \frac{\theta_h^{n+1} - \theta_h^n}{\Delta t} \varphi_{\theta h} \,\mathrm{dx} + \Theta T^{n+1} + (1-\Theta) T^n &= 0,
\end{aligned}
$$

where we define

$$
\begin{aligned}
P^n &:= \int_{\Omega_h} \mathrm{tr}(\nabla \mathbf{v}_h^n) \varphi_h \,\mathrm{dx},\\
V^n &:= \int_{\Omega_h} \rho \left[ (\nabla \mathbf{v}_h^n) \mathbf{v}_h^n - \mathbf{b}^n \right] \cdot \boldsymbol{\varphi}_h \,\mathrm{dx} - \int_{\Omega_h} \mathbf{T}_h^n : \nabla \boldsymbol{\varphi}_h \,\mathrm{dx} + \int_{\Gamma_N} \mathbf{t}^n \cdot \boldsymbol{\varphi}_h \,\mathrm{dS},\\
&\quad \text{where } \mathbf{T}_h^n = -p_h^n \mathbf{I} + \mu_2(\theta_h^n) \left( (\nabla \mathbf{v}_h^n) + (\nabla \mathbf{v}_h^n)^T \right) + G(\theta) (\mathbf{B}_h^n)^d,\\
B^n &:= \int_{\Omega} \left[ (\nabla \mathbf{B}_h^n) \mathbf{v}_h^n - (\nabla \mathbf{v}_h^n) \mathbf{B}_h^n - \mathbf{B}_h^n (\nabla \mathbf{v}_h^n)^T + \frac{G(\theta_h^n)}{\mu_1(\theta_h^n)} \left( \mathbf{B}_h^n (\mathbf{B}_h^n)^d \right) \right] : \boldsymbol{\Phi}_{\boldsymbol{h}} \,\mathrm{dx},\\
T^n &:= \int_{\Omega} \Big[ \rho \Big( c_V (\nabla \theta_h^n) \cdot \mathbf{v}_h^n - r^n \Big) - \frac{\mu_2(\theta_h^n)}{2} \left( (\nabla \mathbf{v}_h^n) + (\nabla \mathbf{v}_h^n)^T \right) : \left( (\nabla \mathbf{v}_h^n) + (\nabla \mathbf{v}_h^n)^T \right) +\\
&\quad \frac{G^2(\theta_h^n)}{2\mu_1(\theta_h^n)} \left( \mathbf{B}_h^n (\mathbf{B}_h^n)^d \right) \Big] \varphi_{\theta h} \,\mathrm{dx} + \int_{\Omega} (k(\theta_h^n) \nabla \theta_h^n) \cdot \nabla \varphi_{\theta h} \,\mathrm{dx} + \int_{\Theta_N} q_N^n \varphi_{\theta h} \,\mathrm{dS}.
\end{aligned}
$$

### 3.2.2 Solving the Discrete Problem

The non-linear system arising from the discrete problem is solved by the Newton method. The block-scheme of the linearised system has a rather general form

$$
\begin{bmatrix} A & B & C & D \\ B^T & 0 & 0 & 0 \\ E & 0 & F & G \\ H & 0 & I & J \end{bmatrix},
$$

where columns and rows correspond to $\mathbf{v}$, $p$, $\mathbf{B}$ and $\theta$, respectively. The linear system in each Newton iteration is solved by the direct solver MUMPS included in PETSc library.

### 3.2.3 Verification of Implementation

To verify our implementation, we compare the results of the simulation with the classical viscoelastic benchmark problem. The test is done for the Oldroyd-B model hence the temperature is not involved and the material coefficients are prescribed constants. The implementation of the model Quad1 differs from the Oldroyd-B only in one term in the evolution equation for extra stress tensor $\mathbf{B}$.

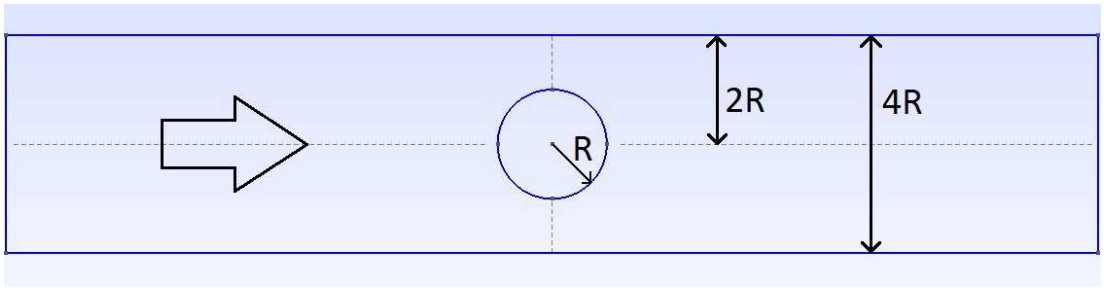



Figure 3.2: The geometry of the problem.

### Problem Description

We consider the planar flow past a cylinder of radius $R$ positioned between two flat plates separated by a distance $H = 4R$. Our computation domain is depicted in (3.2) and consists of a rectangular and a circle in the middle. The width of the rectangular has to be large enough to let the velocity develop its own steady flow profile without respect to an inflow boundary condition. In our case, the width is $20R$. No slip boundary condition for the velocity is assumed on the cylinder and on the walls of the channel and we prescribe parabolic velocity profile of flow rate $Q$ on inflow. It implies the average velocity $U = Q/H$.

We can rewrite the governing equations of the Oldroyd-B model into a dimensionless form

$$\begin{aligned} \operatorname{div} \mathbf{v} &= 0, \\ Re\,\dot{\mathbf{v}} &= -\nabla \tilde{p} + \alpha \Delta \mathbf{v} + \nabla \mathbf{S}, \\ \mathbf{S} + Wi\,\overset{\triangledown}{\mathbf{S}} &= 2(1-\alpha)\mathbf{D}, \end{aligned}$$

where the dimensionless parameters are the Reynold number, the Weissenberg number and the viscosity coefficient

$$\begin{aligned} Re &= \frac{\rho U H}{(\mu_1 + \mu_2)} = \frac{\rho U H}{(\mu_{Tot})}, \\ Wi &= \frac{\mu_1 U}{GR} = \frac{\tau U}{R}, \\ \alpha &= \frac{\mu_2}{\mu_1}. \end{aligned}$$

However, it is convenient to prescribe a viscosity ratio

$$\beta = \frac{\mu_2}{\mu_{Tot}} \in [0, 1),$$

instead of $\alpha$. It is sufficient as the third dimensionless parameter because $\alpha = \beta/(\beta - 1)$. For better orientation in the literature, we present another set of material parameters $\eta_s = \mu_1$ as solvent viscosity, $\eta_p = \mu_2$ as polymeric viscosity and $\tau = \mu_1/G$ as relaxation time (and also $\mu_{Tot} = \mu_1 + \mu_2$). This set of parameters is used also in our reference article for the benchmark problem [8].

In order to be consistent with the reference article, we set $Re = 0$ (to neglect the inertial term), $\beta = 0.59$ and run simulation of the problem for different $Wi$.

| $Wi$ | $M0$ | $M1$ | $M2$ | Reference value [8] |
|---|---|---|---|---|
| 0.1 | 130.195 | 130.299 | 130.371 | 130.36 |
| 0.2 | 126.470 | 126.562 | 126.645 | 126.62 |
| 0.3 | 123.054 | 123.130 | 123.217 | 123.19 |
| 0.4 | - | 120.536 | - | 120.59 |

Table 3.1: The results of the stationary benchmark problem. (the sign "-" means that the algoritm diverges)

| $Wi$ | $M0$ | $M1$ | $M2$ | Reference value [8] |
|---|---|---|---|---|
| 0.1 | 130.195 | 130.300 | 130.372 | 130.36 |
| 0.2 | 126.469 | 126.561 | 126.650 | 126.62 |
| 0.3 | 123.054 | - | 123.253 | 123.19 |
| 0.4 | 120.481 | - | 120.636 | 120.59 |
| 0.5 | 118.587 | - | 118.631 | 118.83 |

Table 3.2: The results of the time-evolutionary benchmark problem. For $Wi \geq 0.6$ algorithm diverges (also the sign "-" means that the algoritm diverges).

The measured quantity is a dimensionless drag coefficient

$$K = \frac{1}{\mu_{Tot} U} \int_{\Gamma_C} \mathbf{Tn} \cdot \mathbf{e}_x \, \mathrm{ds},$$

where $\Gamma_C$ is the boundary of the cylinder, $\mathbf{n}$ the outward unit normal and $\mathbf{e}_x$ unit vector in the $x$ direction. Let us note that the resulting drag coefficient does not depend the choice of $Q$ and $\mu_{Tot}$. We use $Q = 1$ and $\mu_{Tot} = 1$.

**Simulation Results**

The simulation was done with constant coefficients without any dependence on the temperature therefore an evolution equation for temperature was removed from discrete problem. Hence we are testing only the non-temperature part of our implementation. The computation was performed on three computational meshes $M0$, $M1$ and $M2$ depicted in (3.3). The computational mesh $M2$ was designed in such a way that it has comparable number of elements as $M1$ but greater density of elements near the cylinder. The problem is stationary so we set all time derivatives to zero and solve the boundary value problem. Table (3.1) shows the results for low Weissenberg numbers. Unfortunately, for $Wi \geq 0.4$ the Newton method does not converge (the high Weissenberg number problem (HWNP) is the well known numerical issue).

We try to get results for some higher $Wi$ by considering initial and boundary value problem and try to find a stationary state. The time-evolution computation is more successful and diverges for $Wi \geq 0.6$. There is also some difficulty with the mesh $M1$ which we cannot fully explain. However, our aim was the quantitative verification and from this point of view the simulations are successful.

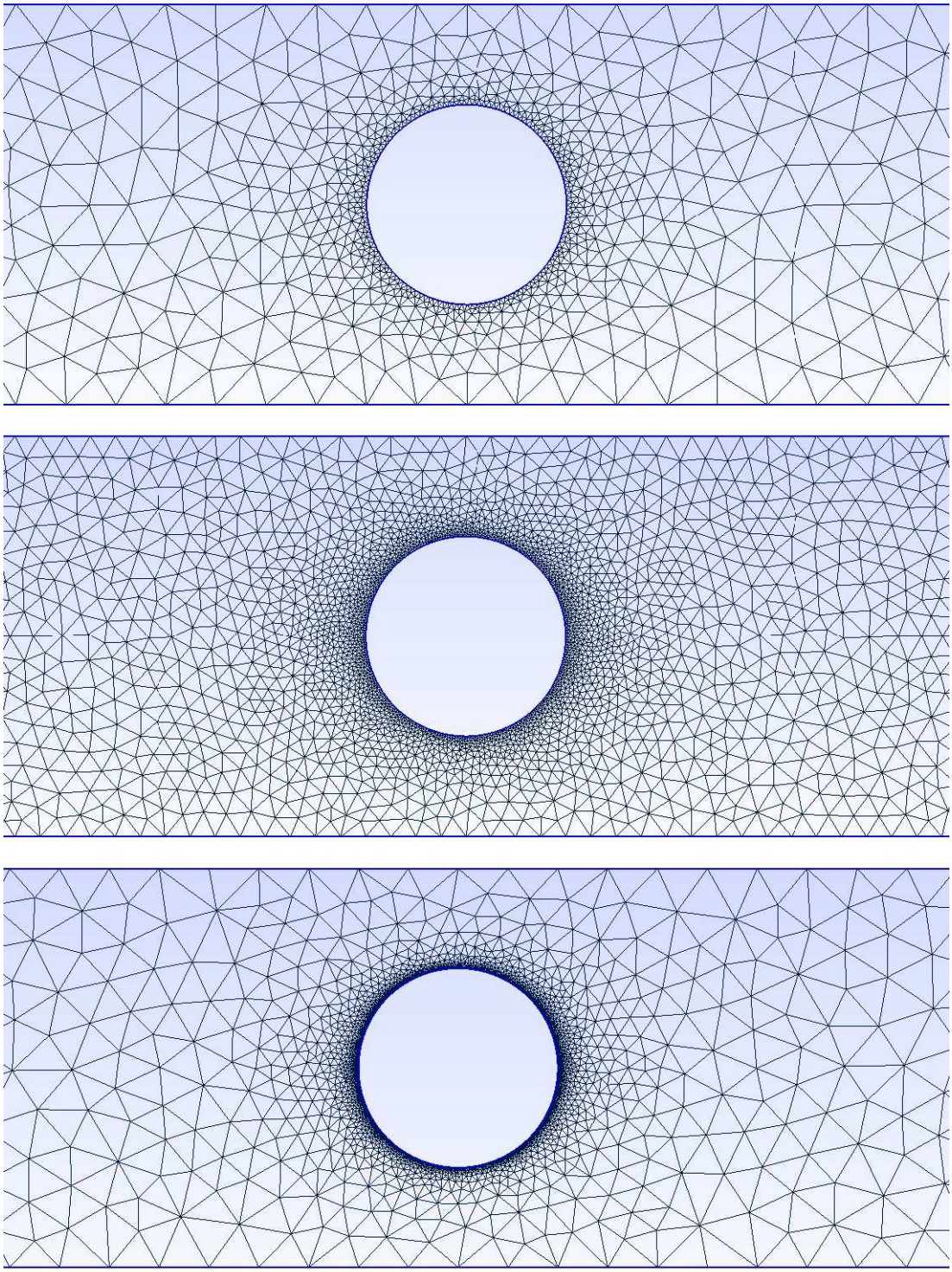


Figure 3.3: Computational meshes $M0$ (1052 elements), $M1$ (3744 elements), $M2$ (5949 elements), respectively from above.

## 3.3 Arbitrary Lagrangian-Eulerian Method

Interesting phenomena of viscoelasticity are connected with the deformation of specimen. So far, our consideration as well as the implementation was done in the Eulerian (spatial) description. It means the material is flowing through the computational domain during the computation. If we want to observe the deformation of the rigid body (fixed set of material points), we need to switch to the Lagrangian description of the motion and connect each point of the computational domain with a fixed material point.

However, when large material deformation occurs, for instance vortices in fluids, the computation suffers from a loss in accuracy, and may even be unable to conclude the calculation, due to excessive distortions of the computational mesh linked to the material. The difficulties caused by the excessive distortion of the finite element grid can be overcome by the Arbitrary Lagrangian-Eulerian (ALE) method.

We present the weak formulation of our models in both Lagrangian and ALE description. We closely follow the section *Computation in the time varying domains* in the doctoral thesis [15].

### 3.3.1 Lagrangian Description

To reformulate the problem from Eulerian to Lagrangian description, we have to introduce a new variable $\mathbf{u}$ as a displacement. Let us denote $\Omega_X$ the material (reference) domain, $\Omega_x$ the spatial (current) domain and $\varphi : X \to x = X + \mathbf{u}$ as one-to-one mapping from $\Omega_X$ into $\Omega_x$. The velocity is defined by

$$\mathbf{v} = \left.\frac{\partial \varphi}{\partial t}\right|_X = \frac{\partial \mathbf{u}}{\partial t},$$

the deformation gradient $\mathbf{F}$ and its Jacobian $\boldsymbol{J}$ are defined as

$$\mathbf{F} = \frac{\partial \varphi}{\partial X} = \mathbf{I} + \nabla_X \mathbf{u},\ \boldsymbol{J} = \det \mathbf{F}.$$

The mapping $\varphi$ is one-to-one thus there exists its inverse $\varphi^{-1} : x \to X = x - \mathbf{u}$ and $\mathbf{F}$ is invertible.

We already have a weak formulation of the problem in the Eulerian description. In order to reformulate the problem to Lagrangian description, we have to express the time and spatial derivatives of Eulerian quantities in the terms of derivatives of Lagrangian quantities. Let us first inspect the transformation of the time derivative of a quantity $\alpha$ ($\alpha$ can be a scalar, vector or tensor - it changes only the meaning of multiplication arising from the chain rule), using the chain rule we have

$$\left.\frac{\partial \alpha}{\partial t}\right|_X = \left.\frac{\mathrm{d}\alpha(\varphi(X,t),t)}{\mathrm{d}t}\right|_X = \left.\frac{\partial \alpha}{\partial t}\right|_x + \left.\frac{\partial \alpha}{\partial x}\,\frac{\partial \varphi}{\partial t}\right|_X = \left.\frac{\partial \alpha}{\partial t}\right|_x + \nabla_x \alpha \cdot \mathbf{v}.$$

Also, we have to transform the gradient of a scalar function[1] $\alpha$

$$\nabla_X\, \alpha = \frac{\partial \alpha(\varphi(X,t),t)}{\partial X} = \frac{\partial \alpha}{\partial x}\frac{\partial \varphi}{\partial X} = (\nabla_x\, \alpha)\mathbf{F},$$

[1]Note that the gradient of a scalar function can be considered to be a row vector. Hence matrix multiplication from the right by the tensor $\mathbf{F}$ makes sense.

which directly implies

$$\nabla_x \alpha = (\nabla_X \alpha)\mathbf{F}^{-1}.$$

By the same derivation it holds for the gradient of a vector function $\mathbf{w}$

$$\nabla_x \mathbf{w} = (\nabla_X \mathbf{w})\mathbf{F}^{-1}.$$

Further, we transform the divergence of the gradient of a scalar function. If we again denote $\mathbf{q} = -k(\theta)\nabla\theta$ and $\tilde{\mathbf{q}} = -k(\theta)\nabla_X\theta\mathbf{F}^{-T}$, we can write

$$\operatorname{div}_x \mathbf{q} = \frac{\partial q_i}{\partial x_i} = \frac{\partial q_i}{\partial X_\alpha} : \frac{\partial X_\alpha}{\partial x_i} = (\nabla_X \mathbf{q}) : \mathbf{F}^{-T},$$

and for a tensor quantity $\mathbf{A} \in \mathbb{R}^{d\times d}$ we have

$$(\operatorname{div}_x \mathbf{A}) = \left((\nabla_X \mathbf{A}) : \mathbf{F}^{-T}\right) \in \mathbb{R}^d.$$

The integrals over $\Omega_x$ are transformed to the integrals over $\Omega_X$ by using integral substitution theorem. We have to take special care of the transformation of the integrals with the divergence. Let us remind the kinematic identity

$$\operatorname{div} \mathbf{qA} = (\nabla\mathbf{q}) : \mathbf{A} + \mathbf{q} \cdot \operatorname{div} \mathbf{A}$$

and Piola identity $\operatorname{div}_X \left((\det \mathbf{F})\mathbf{F}^{-T}\right) = \operatorname{div}_X \left(\boldsymbol{J}\mathbf{F}^{-T}\right) = 0$. We can now write

$$\begin{aligned}
\int_{\Omega_x} \operatorname{div} \mathbf{T} \cdot \mathbf{q} \,\mathrm{d}x &= \int_{\Omega_X} \left(\boldsymbol{J}(\nabla_X \mathbf{T}) : \mathbf{F}^{-T}\right) \cdot \mathbf{q} \,\mathrm{d}X \\
&= \int_{\Omega_X} \left(\boldsymbol{J}(\nabla_X \mathbf{T})\mathbf{F}^{-T} + \mathbf{T} \operatorname{div}_X (\boldsymbol{J}\mathbf{F}^{-T})\right) \cdot \mathbf{q} \,\mathrm{d}X \\
&= \int_{\Omega_X} \operatorname{div}_X (\boldsymbol{J}\mathbf{T}\mathbf{F}^{-T}) \cdot \mathbf{q} \,\mathrm{d}X
\end{aligned}$$

and

$$\begin{aligned}
\int_{\Omega_x} \operatorname{div}_x \mathbf{q}\, q_\theta \,\mathrm{d}x &= \int_{\Omega_X} \left(\boldsymbol{J}(\nabla_X \mathbf{q}) : \mathbf{F}^{-T}\right) q_\theta \,\mathrm{d}X \\
&= \int_{\Omega_X} \left(\boldsymbol{J}(\nabla_X \mathbf{q})\mathbf{F}^{-T} + \mathbf{q} \operatorname{div}_X (\boldsymbol{J}\mathbf{F}^{-T})\right) q_\theta \,\mathrm{d}X \\
&= \int_{\Omega_X} \operatorname{div}_X (\boldsymbol{J}\mathbf{q}\mathbf{F}^{-T}) q_\theta \,\mathrm{d}X \\
&= -\int_{\Omega_X} \operatorname{div}_X \left(\boldsymbol{J}k(\theta)(\nabla_X\theta\mathbf{F}^{-1})\mathbf{F}^{-T}\right) q_\theta \,\mathrm{d}X.
\end{aligned}$$

Now we are prepared to rewrite the weak formulation of the derived models in the Lagrangian description. We suppose $\mathbf{u} \in L^\infty(0,T;W^{1,2}(\Omega_X))$ and the initial condition $\mathbf{u}(t=0) = 0$. For the sake of simplicity let us make abbreviations

$$\begin{aligned}
U &:= L^\infty(0,T;W^{1,2}(\Omega_X)), \\
\mathbf{D}_X &:= \frac{1}{2}\left((\nabla\mathbf{v})\mathbf{F}^{-1} + \mathbf{F}^{-T}(\nabla\mathbf{v})^T\right), \\
\tilde{\mathbf{t}} &:= \left(\boldsymbol{J}\mathbf{T}\mathbf{F}^{-T}\right)\mathbf{n}_X, \text{ on } \Gamma_N, \\
\tilde{\theta}_N &:= (\boldsymbol{J}k(\theta)\nabla\theta\mathbf{F}^{-1}\mathbf{F}^{-T}) \cdot \mathbf{n}_X, \text{ on } \Theta_N,
\end{aligned}$$

where $\tilde{\mathbf{t}}$ and $\tilde{\theta}_N$ represent standard Neumann boundary conditions prescribed on the boundary of material domain $\Omega_X$. Since we are dealing with an incompressible deformation, instead of

$$\int_{\Omega_X} \boldsymbol{J}\mathrm{tr}\left((\nabla\mathbf{v})\mathbf{F}^{-1}\right)\varphi\,\mathrm{d}X = 0$$

we can write

$$\int_{\Omega_X} (\boldsymbol{J}-1)\,\varphi\,\mathrm{d}X = 0.$$

**T-Oldroyd-B**

The weak formulation for the model T-Oldroyd-B is transformed into the Lagrangian description in $\Omega_X$ as follows:

The quintuple $(\mathbf{v}, p, \mathbf{B}, \theta, \mathbf{u}) \in V \times P \times B \times \Theta \times U$, such that $\mathbf{v} - \tilde{\mathbf{v}} \in V_0$ and $\theta - \tilde{\theta} \in \Theta_0$, is the weak solution of the model T-Oldroyd-B in $\Omega \subset \mathbb{R}^d$ if

$$\int_{\Omega_X}\left(\frac{\partial\mathbf{u}}{\partial t} - \mathbf{v}\right)\cdot\boldsymbol{\varphi}_{\mathbf{u}}\,\mathrm{d}X = 0,$$

$$\int_{\Omega_X}(\boldsymbol{J}-1)\,\varphi\,\mathrm{d}X = 0,$$

$$\int_{\Omega_X}\boldsymbol{J}\rho\left[\frac{\partial\mathbf{v}}{\partial t} - \mathbf{b}\right]\cdot\boldsymbol{\varphi}\,\mathrm{d}X - \int_{\Omega_X}(\boldsymbol{J}\mathbf{T}\mathbf{F}^{-T}) : \nabla\boldsymbol{\varphi}\,\mathrm{d}X + \int_{\Gamma_N}\tilde{\mathbf{t}}\cdot\boldsymbol{\varphi}\,\mathrm{dS} = 0,$$

$$\mathbf{T} = -p\mathbf{I} + 2\mu_2(\theta)\mathbf{D}_X + G(\theta)(\mathbf{B}-\mathbf{I}),$$

$$\int_{\Omega_X}\boldsymbol{J}\left[\frac{\partial\mathbf{B}}{\partial t} - (\nabla\mathbf{v})\mathbf{F}^{-1}\mathbf{B} - \mathbf{B}\mathbf{F}^{-T}(\nabla\mathbf{v})^T + \frac{G(\theta)}{\mu_1(\theta)}(\mathbf{B}-\mathbf{I})\right] : \boldsymbol{\Phi}\,\mathrm{d}X = 0,$$

$$\int_{\Omega_X}\boldsymbol{J}\left[\rho\left(c_V\frac{\partial\theta}{\partial t} - r\right) - 2\mu_2(\theta)\mathbf{D}_X : \mathbf{D}_X + \frac{G^2(\theta)}{2\mu_1(\theta)}\left(\mathrm{tr}\mathbf{B} + \mathrm{tr}(\mathbf{B}^{-1}) - 2d\right)\right]\varphi_\theta\,\mathrm{d}X +$$

$$\int_{\Omega_X}(\boldsymbol{J}k(\theta)\nabla\theta\mathbf{F}^{-1}\mathbf{F}^{-T})\cdot\nabla\varphi_\theta\,\mathrm{d}X + \int_{\Theta_N}\tilde{q}_N\varphi_\theta\,\mathrm{dS} = 0,$$

is satisfied for all $(\boldsymbol{\varphi}, \varphi, \boldsymbol{\Phi}, \varphi_\theta, \boldsymbol{\varphi_u}) \in V_0 \times P \times B \times \Theta_0 \times U$ and almost all $t \in (0,T)$, where $\tilde{\mathbf{v}}|_{\Gamma_D} = \mathbf{v}_D$, $\tilde{\theta}|_{\Theta_D} = \theta_D$ and $r \in L^2(0,T;L^2(\Omega))$, $\mathbf{b} \in L^2(0,T;L^2(\Omega))^d$.

**T-Quad1**

The weak formulation for the model T-Oldroyd-B is transformed into the Lagrangian description in $\Omega_X$ as follows:

The quintuple $(\mathbf{v}, p, \mathbf{B}, \theta, \mathbf{u}) \in V \times P \times B \times \Theta \times U$, such that $\mathbf{v} - \tilde{\mathbf{v}} \in V_0$ and

$\theta - \tilde{\theta} \in \Theta_0$, is the weak solution of the model T-Oldroyd-B in $\Omega \subset \mathbb{R}^d$ if

$$\int_{\Omega_X} \left( \frac{\partial \mathbf{u}}{\partial t} - \mathbf{v} \right) \cdot \boldsymbol{\varphi}_{\mathbf{u}} \, \mathrm{d}X = 0,$$

$$\int_{\Omega_X} (\boldsymbol{J} - 1) \, \varphi \, \mathrm{d}X = 0,$$

$$\int_{\Omega_X} \boldsymbol{J} \rho \left[ \frac{\partial \mathbf{v}}{\partial t} - \mathbf{b} \right] \cdot \boldsymbol{\varphi} \, \mathrm{d}X - \int_{\Omega_X} (\boldsymbol{J} \mathbf{T} \mathbf{F}^{-T}) : \nabla \boldsymbol{\varphi} \, \mathrm{d}X + \int_{\Gamma_N} \tilde{\mathbf{t}} \cdot \boldsymbol{\varphi} \, \mathrm{dS} = 0,$$

$$\mathbf{T} = -p\mathbf{I} + 2\mu_2(\theta)\mathbf{D}_X + G(\theta)\mathbf{B}^d,$$

$$\int_{\Omega_X} \boldsymbol{J} \left[ \frac{\partial \mathbf{B}}{\partial t} - (\nabla \mathbf{v})\mathbf{F}^{-1}\mathbf{B} - \mathbf{B}\mathbf{F}^{-T}(\nabla \mathbf{v})^T + \frac{G(\theta)}{\mu_1(\theta)}(\mathbf{B}\mathbf{B}^d) \right] : \boldsymbol{\Phi} \, \mathrm{d}X = 0,$$

$$\int_{\Omega_X} \boldsymbol{J} \left[ \rho \left( c_V \frac{\partial \theta}{\partial t} - r \right) - 2\mu_2(\theta)\mathbf{D}_X : \mathbf{D}_X + \frac{G^2(\theta)}{2\mu_1(\theta)} \left( \mathbf{B}\mathbf{B}^d \right) \right] \varphi_\theta \, \mathrm{d}X +$$

$$\int_{\Omega_X} (\boldsymbol{J} k(\theta) \nabla\theta \mathbf{F}^{-1}\mathbf{F}^{-T}) \cdot \nabla \varphi_\theta \, \mathrm{d}X + \int_{\Theta_N} \tilde{q}_N \varphi_\theta \, \mathrm{dS} = 0,$$

is satisfied for all $(\boldsymbol{\varphi}, \varphi, \boldsymbol{\Phi}, \varphi_\theta, \boldsymbol{\varphi_u}) \in V_0 \times P \times B \times \Theta_0 \times U$ and almost all $t \in (0, T)$, where $\tilde{\mathbf{v}}|_{\Gamma_D} = \mathbf{v}_D$, $\tilde{\theta}|_{\Theta_D} = \theta_D$ and $r \in L^2(0, T; L^2(\Omega))$, $\mathbf{b} \in L^2(0, T; L^2(\Omega))^d$.

### 3.3.2 ALE Description

Using the Lagrangian description to solve the problem of deforming a piece of material is sufficient in many applications, especially in solid mechanics. However, we are dealing with viscoelastic materials with temperature dependent material coefficients and for high temperatures the specimen can behave like a fluid and some problems can arise during the computation due to the large motion of the material. Therefore we need to use something between the Lagrangian and Eulerian description and Arbitrary Lagrangian-Eulerian (ALE) description is the right choice. Details about the ALE method can be found in [5].

The method is based on the arbitrary configuration "somewhere between" the material and spatial configurations. Precisely speaking, let $\Omega_\chi \subset \mathbb{R}^d$ and

$$\hat{\phi} : \chi \to x = \chi + \hat{\mathbf{u}}$$

maps $\Omega_\chi$ into $\Omega_x$. The quantity $\hat{\mathbf{u}}$ is called an arbitrary deformation. If the time derivative of $\hat{\mathbf{u}}$ is equal to $\mathbf{v}$ then arbitrary configuration merges with material configuration, $\Omega_\chi = \Omega_X$. Instead of this, we only need to have the material points on the boundary $\partial\Omega_\chi$. Inside the domain $\Omega_\chi$, we just need to have a unique solution for $\hat{\mathbf{u}}$. For simplicity's sake we use a Laplace equation, i.e.

$$\begin{aligned} \frac{\partial \hat{\mathbf{u}}}{\partial t} &= \mathbf{v} \quad \text{on } \partial\Omega_\chi, \\ -\Delta_\chi \hat{\mathbf{u}} &= 0 \quad \text{inside } \Omega_\chi. \end{aligned}$$

In a standard way we define the analogue to the deformation gradient and its Jacobian by

$$\hat{\mathbf{F}} = \frac{\partial \hat{\varphi}}{\partial \chi} = \mathbf{I} + \nabla_\chi \hat{\mathbf{u}}, \quad \hat{J} = \det \hat{\mathbf{F}}.$$

The transformations of all quantities (e.g. $\nabla_\chi \mathbf{v}$) are the same as for the Lagrangian description, except for the transformation of the material time derivative. If we proceeded in the same way as for the Lagrangian description, we would obtain

$$\left.\frac{\partial \alpha}{\partial t}\right|_\chi = \left.\frac{\mathrm{d}\alpha(\hat{\varphi}(\chi,t),t)}{\mathrm{d}t}\right|_\chi = \left.\frac{\partial \alpha}{\partial t}\right|_x + \left.\frac{\partial \alpha}{\partial x}\,\frac{\partial \hat{\varphi}}{\partial t}\right|_\chi = \left.\frac{\partial \alpha}{\partial t}\right|_x + \nabla_x \alpha \cdot \frac{\partial \hat{\mathbf{u}}}{\partial t}. \tag{3.3.1}$$

But we need to have $\mathbf{v}$ instead of the time derivation of $\hat{\mathbf{u}}$ in the last term of (3.3.1). Hence using (3.3.1) and the transformation rule for $\nabla_x \alpha$ we consider

$$\begin{aligned}
\left.\frac{\partial \alpha}{\partial t}\right|_x + \nabla_x \alpha \cdot \mathbf{v} &= \left.\frac{\partial \alpha}{\partial t}\right|_\chi + \nabla_x \alpha \cdot \left(\mathbf{v} - \frac{\partial \hat{\mathbf{u}}}{\partial t}\right) \\
&= \left.\frac{\partial \alpha}{\partial t}\right|_\chi + (\nabla_\chi \alpha)\hat{\mathbf{F}}^{-1} \cdot \left(\mathbf{v} - \frac{\partial \hat{\mathbf{u}}}{\partial t}\right) \\
&= \left.\frac{\partial \alpha}{\partial t}\right|_\chi + \nabla_\chi \alpha \cdot \left(\hat{\mathbf{F}}^{-1}\left(\mathbf{v} - \frac{\partial \hat{\mathbf{u}}}{\partial t}\right)\right).
\end{aligned}$$

Now we are able to rewrite the weak formulation of the derived models in the ALE description. As for the Lagrangian description, let us assume the initial and boundary conditions

$$\begin{aligned}
\hat{\mathbf{u}}(t=0) &= 0, \\
\frac{\partial \hat{\mathbf{u}}}{\partial t} &= \mathbf{v}, \text{ on } \partial\Omega_\chi,
\end{aligned}$$

and abbreviate

$$\begin{aligned}
U &:= L^\infty(0,T;W^{1,2}(\Omega_\chi)), \\
\mathbf{D}_\chi &:= \frac{1}{2}\left((\nabla \mathbf{v})\hat{\mathbf{F}}^{-1} + \hat{\mathbf{F}}^{-T}(\nabla \mathbf{v})^T\right), \\
\hat{\mathbf{t}} &:= \left(\hat{\boldsymbol{J}}\hat{\mathbf{T}}\hat{\mathbf{F}}^{-T}\right)\mathbf{n}_\chi, \text{ on } \Gamma_N, \\
\hat{\theta}_N &:= (\hat{\boldsymbol{J}} k(\theta)\nabla\theta\hat{\mathbf{F}}^{-1}\hat{\mathbf{F}}^{-T}) \cdot \mathbf{n}_\chi, \text{ on } \Theta_N, \\
\frac{\mathrm{D}\alpha}{\mathrm{D}} &:= \frac{\partial \alpha}{\partial t} + \nabla \alpha \cdot \left(\hat{\mathbf{F}}^{-1}\left(\mathbf{v} - \frac{\partial \hat{\mathbf{u}}}{\partial t}\right)\right)
\end{aligned}$$

where $\hat{\mathbf{t}}$ and $\hat{\theta}_N$ represent the standard Neumann boundary conditions prescribed on the boundary of material domain $\Omega_\chi$.

**Penalty term** If the boundary condition

$$\frac{\partial \hat{\mathbf{u}}}{\partial t} = \mathbf{v}, \text{ on } \partial\Omega_\chi \tag{3.3.2}$$

cannot be prescribed, it can be replaced in the week formulation by a penalty term

$$\int_{\partial\Omega_\chi} \alpha\left(\mathbf{v} - \frac{\partial \hat{\mathbf{u}}}{\partial t}\right) \cdot \boldsymbol{\varphi}_{\hat{\mathbf{u}}}\,\mathrm{d}S = 0, \tag{3.3.3}$$

which can be understood as an auxiliary force trying to keep the condition 3.3.2. The penalty $\alpha$ determines how strong the force is.

**T-Oldroyd-B**

The weak formulation for the model T-Oldroyd-B is transformed into the Lagrangian description in $\Omega_\chi$ as follows:

The quintuple $(\mathbf{v}, p, \mathbf{B}, \theta, \hat{\mathbf{u}}) \in V \times P \times B \times \Theta \times U$, such that $\mathbf{v} - \tilde{\mathbf{v}} \in V_0$ and $\theta - \tilde{\theta} \in \Theta_0$, is the weak solution of the model T-Oldroyd-B in $\Omega \subset \mathbb{R}^d$ if

$$\int_{\Omega_\chi} \nabla \hat{\mathbf{u}} \cdot \nabla \boldsymbol{\varphi}_{\hat{\mathbf{u}}} \,\mathrm{d}\chi = 0,$$

$$\int_{\partial\Omega_\chi} \alpha \left( \mathbf{v} - \frac{\partial \hat{\mathbf{u}}}{\partial t} \right) \cdot \boldsymbol{\varphi}_{\hat{\mathbf{u}}} \,\mathrm{d}S = 0,$$

$$\int_{\Omega_\chi} \hat{\boldsymbol{J}} \mathrm{tr} \left( (\nabla \mathbf{v}) \hat{\mathbf{F}}^{-1} \right) \varphi \,\mathrm{d}\chi = 0,$$

$$\int_{\Omega_\chi} \hat{\boldsymbol{J}} \rho \left[ \frac{\mathrm{D}\mathbf{v}}{\mathrm{D}t} - \mathbf{b} \right] \cdot \boldsymbol{\varphi} \,\mathrm{d}\chi - \int_{\Omega_\chi} (\hat{\boldsymbol{J}} \hat{\mathbf{T}} \hat{\mathbf{F}}^{-T}) : \nabla \boldsymbol{\varphi} \,\mathrm{d}\chi + \int_{\Gamma_N} \hat{\mathbf{t}} \cdot \boldsymbol{\varphi} \,\mathrm{dS} = 0,$$

$$\hat{\mathbf{T}} = -p\mathbf{I} + 2\mu_2(\theta)\mathbf{D}_\chi + G(\theta)(\mathbf{B} - \mathbf{I}),$$

$$\int_{\Omega_\chi} \hat{\boldsymbol{J}} \left[ \frac{\mathrm{D}\mathbf{B}}{\mathrm{D}t} - (\nabla \mathbf{v}) \hat{\mathbf{F}}^{-1} \mathbf{B} - \mathbf{B} \hat{\mathbf{F}}^{-T} (\nabla \mathbf{v})^T + \frac{G(\theta)}{\mu_1(\theta)} (\mathbf{B} - \mathbf{I}) \right] : \boldsymbol{\Phi} \,\mathrm{d}\chi = 0,$$

$$\int_{\Omega_\chi} \hat{\boldsymbol{J}} \left[ \rho \left( c_V \frac{\mathrm{D}\theta}{\mathrm{D}t} - r \right) - 2\mu_2(\theta) \mathbf{D}_\chi : \mathbf{D}_\chi + \frac{G^2(\theta)}{2\mu_1(\theta)} \left( \mathrm{tr}\mathbf{B} + \mathrm{tr}(\mathbf{B}^{-1}) - 2d \right) \right] \varphi_\theta \,\mathrm{d}\chi +$$

$$\int_{\Omega_\chi} (\hat{\boldsymbol{J}} k(\theta) \nabla\theta \hat{\mathbf{F}}^{-1} \hat{\mathbf{F}}^{-T}) \cdot \nabla \varphi_\theta \,\mathrm{d}\chi + \int_{\Theta_N} \hat{q}_N \varphi_\theta \,\mathrm{dS} = 0,$$

is satisfied for all $(\boldsymbol{\varphi}, \varphi, \boldsymbol{\Phi}, \varphi_\theta, \boldsymbol{\varphi}_{\hat{\mathbf{u}}}) \in V_0 \times P \times B \times \Theta_0 \times U$ and almost all $t \in (0, T)$, where $\tilde{\mathbf{v}}|_{\Gamma_D} = \mathbf{v}_D$, $\tilde{\theta}|_{\Theta_D} = \theta_D$ and $r \in L^2(0, T; L^2(\Omega))$, $\mathbf{b} \in L^2(0, T; L^2(\Omega))^d$.

**T-Quad1**

The weak formulation for the model T-Oldroyd-B is transformed into the Lagrangian description in $\Omega_\chi$ as follows:

The quintuple $(\mathbf{v}, p, \mathbf{B}, \theta, \hat{\mathbf{u}}) \in V \times P \times B \times \Theta \times U$, such that $\mathbf{v} - \tilde{\mathbf{v}} \in V_0$ and $\theta - \tilde{\theta} \in \Theta_0$, is the weak solution of the model T-Oldroyd-B in $\Omega \subset \mathbb{R}^d$ if

$$\int_{\Omega_\chi} \nabla \hat{\mathbf{u}} \cdot \nabla \boldsymbol{\varphi}_{\hat{\mathbf{u}}} \,\mathrm{d}\chi = 0,$$

$$\int_{\partial\Omega_\chi} \alpha \left( \mathbf{v} - \frac{\partial \hat{\mathbf{u}}}{\partial t} \right) \cdot \boldsymbol{\varphi}_{\hat{\mathbf{u}}} \,\mathrm{d}S = 0,$$

$$\int_{\Omega_\chi} \hat{\boldsymbol{J}} \mathrm{tr} \left( (\nabla \mathbf{v}) \hat{\mathbf{F}}^{-1} \right) \varphi \,\mathrm{d}\chi = 0,$$

$$\int_{\Omega_\chi} \hat{\boldsymbol{J}} \rho \left[ \frac{\mathrm{D}\mathbf{v}}{\mathrm{D}t} - \mathbf{b} \right] \cdot \boldsymbol{\varphi} \,\mathrm{d}\chi - \int_{\Omega_\chi} (\hat{\boldsymbol{J}} \hat{\mathbf{T}} \hat{\mathbf{F}}^{-T}) : \nabla \boldsymbol{\varphi} \,\mathrm{d}\chi + \int_{\Gamma_N} \hat{\mathbf{t}} \cdot \boldsymbol{\varphi} \,\mathrm{dS} = 0,$$

$$\hat{\mathbf{T}} = -p\mathbf{I} + 2\mu_2(\theta)\mathbf{D}_\chi + G(\theta)\mathbf{B}^d,$$

$$\int_{\Omega_\chi} \hat{\boldsymbol{J}} \left[ \frac{\mathrm{D}\mathbf{B}}{\mathrm{D}t} - (\nabla \mathbf{v}) \hat{\mathbf{F}}^{-1} \mathbf{B} - \mathbf{B} \hat{\mathbf{F}}^{-T} (\nabla \mathbf{v})^T + \frac{G(\theta)}{\mu_1(\theta)} (\mathbf{B}\mathbf{B}^d) \right] : \boldsymbol{\Phi} \,\mathrm{d}\chi = 0,$$

$$\int_{\Omega_\chi} \hat{\boldsymbol{J}} \left[ \rho \left( c_V \frac{\mathrm{D}\theta}{\mathrm{D}t} - r \right) - 2\mu_2(\theta) \mathbf{D}_\chi : \mathbf{D}_\chi + \frac{G^2(\theta)}{2\mu_1(\theta)} \left( \mathbf{B}\mathbf{B}^d \right) \right] \varphi_\theta \,\mathrm{d}\chi +$$

$$\int_{\Omega_\chi} (\hat{\boldsymbol{J}} k(\theta) \nabla\theta \hat{\mathbf{F}}^{-1} \hat{\mathbf{F}}^{-T}) \cdot \nabla \varphi_\theta \,\mathrm{d}\chi + \int_{\Theta_N} \hat{q}_N \varphi_\theta \,\mathrm{dS} = 0,$$

is satisfied for all $(\boldsymbol{\varphi}, \varphi, \boldsymbol{\Phi}, \varphi_\theta, \boldsymbol{\varphi}_{\hat{\mathbf{u}}}) \in V_0 \times P \times B \times \Theta_0 \times U$ and almost all $t \in (0, T)$, where $\tilde{\mathbf{v}}|_{\Gamma_D} = \mathbf{v}_D$, $\tilde{\theta}|_{\Theta_D} = \theta_D$ and $r \in L^2(0, T; L^2(\Omega))$, $\mathbf{b} \in L^2(0, T; L^2(\Omega))^d$.

### 3.3.3 Verification of the Implementation

For the verification of the code written in Lagrangian or ALE formulation, we decided to perform uni-axial stress simulation on a rectangular piece of Neo-Hookean material. Neo-Hookean material can be obtained from the Oldroy-B model (or also Quad1 model) by considering a limit case $\mu_2 \to 0$ and $\mu_1 \to \infty$. After applying the stress, the rate of elongation $\epsilon$ of the specimen is compared with an analytic solution. We define $\epsilon$ by the relation

$$l_e = \epsilon\, l, \tag{3.3.4}$$

where $l$ and $l_e$ are initial and final length of the specimen, respectively. Inertia effects are neglected by setting $\rho = 0$.

#### Problem description

The considered geometry and boundary conditions are depicted on 3.4. It consists of the a rectangle of height $h = 2$ and length $l = 4$. Let us denote $\mathbf{P}$ as the first Piola-Kirchhoff tensor. Let us recall the relation between the Cauchy stress tensor $\mathbf{T}$ and the first Piola-Kirchhoff tensor $\mathbf{P}$

$$\mathbf{P} = J\mathbf{T}\mathbf{F}^{-T}. \tag{3.3.5}$$

On the top and the bottom of the rectangle so called *do nothing* boundary condition $\mathbf{Pn} = 0$ is prescribed. The right hand side of the specimen is pulled by a constant force $\mathbf{F}$. Therefore we prescribe a constant boundary condition $\mathbf{Pn} = (\mathbf{f}, 0)$ on the right hand side of the rectangle, where $\mathbf{f}\,h = \mathbf{F}$ is the desired pull force. Note that $\mathbf{P}$ and $\mathbf{n}$ are in the reference configuration. At the wall, we only demand $v_x = 0$ (instead of $\mathbf{v} = 0$) to allow an uniaxial deformation of the specimen.

#### Reduction to Neo-Hookean Material

Let us show that Oldroyd-B model (and also Quad1 model) reduces to Neo-Hookean material if we consider a limit case $\mu_2 \to 0$ and $\mu_1 \to \infty$. Constitutive relation for both models reduces to

$$\begin{aligned} \mathbf{T} &= -p\mathbf{I} + G\left(\mathbf{B}_{\kappa_p(t)} - \mathbf{I}\right) \\ \overset{\triangledown}{\mathbf{B}}_{\kappa_p(t)} &= 0. \end{aligned}$$

From 2.2.2 we have

$$0 = \overset{\triangledown}{\mathbf{B}}_{\kappa_p(t)} = -2\mathbf{F}_{\kappa_p(t)}\mathbf{D}_{\kappa_p(t)}\mathbf{F}^T_{\kappa_p(t)}.$$

Hence we conclude that

$$\mathbf{D}_{\kappa_p(t)} = 0,$$

which implies

$$\mathbf{B}_{\kappa_p(t)} = \mathbf{B}.$$

In other words, extra stress tensor $\mathbf{B}_{\kappa_p(t)}$ is the left Cauchy-Green tensor of the whole deformation. Therefore, we obtain the constitutive relation for an incompressible Neo-Hookean material

$$\mathbf{T} = -p\mathbf{I} + G\left(\mathbf{B} - \mathbf{I}\right). \tag{3.3.6}$$

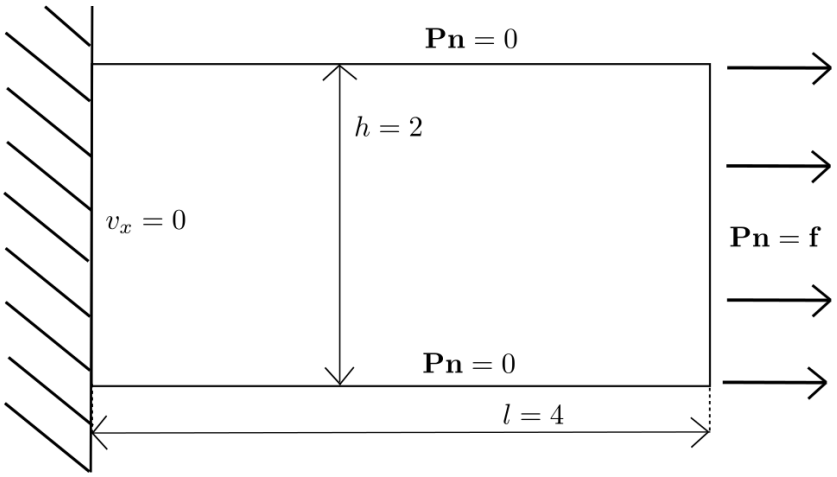



Figure 3.4: Geometry and boundary conditions of the problem.

**Analytic solution**

From 3.3.6, we obtain the constitutive relation in the Lagrangian description

$$\mathbf{P} = J\left(-p\mathbf{F}^{-T} + G(\mathbf{F} + \mathbf{F}^{-T})\right)$$

using the transformation rule 3.3.5. Let us denote a displacement as $\mathbf{u} = (u, v)$. Due to the geometry of the problem we can assume an uni-axial deformation $\mathbf{u} = (u(x), v(y))$, hence the deformation gradient takes the form

$$\mathbf{F} = \begin{bmatrix} \lambda & 0 \\ 0 & \frac{1}{\lambda} \end{bmatrix},$$

where $\lambda = 1 + u_x$ and $u_x$ denotes the partial derivative $u$ by $x$. Note that the rate of elongation $\epsilon$ defined in (3.3.4) and $u_x$ are equal in this case because we assume $\lambda \neq 0$ to be constant in the whole domain. This assumption allows us to write

$$\mathbf{P} = -p \begin{bmatrix} \frac{1}{\lambda} & 0 \\ 0 & \lambda \end{bmatrix} + G \begin{bmatrix} \lambda - \frac{1}{\lambda} & 0 \\ 0 & \frac{1}{\lambda} - \lambda \end{bmatrix} \tag{3.3.7}$$

because $J = 1$ for an uni-axial deformation. The boundary condition *do nothing* $\mathbf{Pn} = 0$ for $\mathbf{n} = (0, \pm 1)$ gives us a relation for the pressure

$$p = G\frac{1 - \lambda^2}{\lambda^2}. \tag{3.3.8}$$

We also suppose $p$ to be constant in the whole domain. The second boundary condition $\mathbf{Pn} = (f, 0)$ for $\mathbf{n} = (1, 0)$ gives

$$f = -G\frac{1 - \lambda^2}{\lambda^3} + G\frac{\lambda^2 - 1}{\lambda},$$

which leads to

$$\lambda^4 = \frac{f}{G}\lambda^3 + 1. \tag{3.3.9}$$

Now we are able to analytically compute the rate of elongation $u_x$ of the specimen depending on the density of pulling force $f$ and the Young's modulus $G$ by the relation

$$u_x = \lambda_1 - 1,$$

where $\lambda_1$ is the positive real root of the equation (3.3.9). This definition is correct due to the next lemma.

**Lemma 3.3.1.** *For $a \in \mathbb{R}$, $a \geq 0$ there exist only one positive real root of the equation*

$$\lambda^4 = a\lambda^3 + 1.$$

*Proof.* Let us denote $Q(\lambda) := \lambda^4 - a\lambda^3 - 1$. Clearly

$$Q(0) = -1 \quad \text{and} \quad \lim_{\lambda \to \pm\infty} Q(\lambda) = \infty. \tag{3.3.10}$$

The derivative of $Q(\lambda)$ reads

$$\frac{\mathrm{d}Q(\lambda)}{\mathrm{d}\lambda} = \lambda^2(4\lambda - 3a),$$

which means the only stationary points of $Q(\lambda)$ are $\lambda_n = 0$ and $\lambda_s = 3a/4$. Furthermore, according to the sign of the derivative, $Q(\lambda)$ is non-increasing on the interval $[-\infty, \lambda_s]$, non-descending on the interval $[\lambda_s, \infty]$ and also strictly monotonous for all $\lambda \in \mathbb{R}\{\lambda_n, \lambda_s\}$. This monotony, (3.3.10) and Darboux intermediate value property of polynomials imply exactly one positive and one negative root of $Q(\lambda)$. □

### Simulation Results

The problem looks like a stationary problem but we need to test time-evolutionary code. If we start simulation with a relaxed specimen and apply the pulling force at one moment, the change of length of the specimen is instant because of absence of dissipation in the Neo-Hookean model. If the pulling force is large, this jump is bad for a time stepping scheme. One has to either add an auxiliary dissipation (which does not change the result) or increase the pulling force slowly enough until it reaches the desired value. We choose the second approach and introduce the quantity $\Delta F$ as the force increment. Let us point out that results do not depend on the size of computational mesh because the deformation is really uni-axial and has always a perfect rectangular shape.

**Lagrangian Description** In the case of Lagrangian description, simulation results shown in the table (3.3) are satisfactory for the force increment $\Delta F = 0.01$ and Young's modulus $G = 1$.

| Force $F$ | Elongation rate $\epsilon$ | Anal. value of $u_x$ |
|---|---|---|
| 0.01 | 0.002509 | 0.002509 |
| 0.1 | 0.025968 | 0.025970 |
| 0.5 | 0.152701 | 0.152777 |
| 1.0 | 0.379697 | 0.380278 |
| 2.0 | 1.101999 | 1.106919 |

Table 3.3: Results of the benchmark problem for the force increment $\Delta F = 0.01$ and Young's modulus $G = 1$.)

| Force $F$ | Penalty $\alpha$ | $\epsilon$ for $\Delta F = 0.01$ | $\epsilon$ for $\Delta F = 0.001$ | Anal. value of $u_x$ |
|---|---|---|---|---|
| 1.0 | 10000 | 0.379518 | 0.380162 | 0.380278 |
| | 1000 | 0.379135 | 0.379775 | 0.380278 |
| | 100 | 0.375385 | 0.375984 | 0.380278 |
| | 10 | 0.344113 | 0.344399 | 0.380278 |
| 2.0 | 10000 | 1.097126 | 1.105375 | 1.106919 |

Table 3.4: Results of the benchmark problem for ALE description for Young's modulus $G = 1$.

**ALE Description** In comparison with Lagrangian description, our implementation of ALE description has another parameter - penalty $\alpha$ (defined in (3.3.3)). The convergence of $\epsilon$ with respect to penalty $\alpha$ is shown in the table (3.4) for the force $F = 1$, Young's modulus $G = 1$ and two force increment steps $\Delta F = 0.01$ and $\Delta F = 0.001$. Again, the results are satisfactory.

## 3.4 Temperature Benchmark: Couette Flow

In this section, we verify the implementation of the temperature dependent model T-Oldroyd-B on the Cylindrical Couette steady flow problem. The influence of the temperature is demonstrated through temperature dependent Young's modulus $G(\theta)$. For simplicity's sake, we assume the temperature dependence to be exponential

$$G(\theta) = G_0 e^{\alpha(\theta - \theta_R)},$$

where $G_0 > 0$, $\alpha$ are constants and $\theta_R$ is a reference temperature. Other material coefficients $\mu_1$, $\mu_2$ and $\kappa$ remain constant.

To find an analytic solution of the problem, the governing equations are transformed into the cylindrical coordinates. We use a numerical integration to evaluate a semi-analytic solution and compare results of simulation with it.

### 3.4.1 Problem description

The Cylindrical Couette flow takes place between two concentric infinite cylinders of radii $R_1 < R_2$. The inner and outer cylinders (and also the fluid on the boundaries) rotate with the constant angular velocities $\Omega_1$ and $\Omega_2$, respectively. The problem is originally 3D, but for a low velocities we can assume the symmetry in the $z$ axis, hence we are interested in the 2D problem - plane section for any $z = \text{const}$, which is depicted in Figure (3.5), where $\mathbf{g}_{\hat{r}}$ and $\mathbf{g}_{\hat{\varphi}}$ are normed basis

vectors of the cylindrical coordinates. We solve the full 3D problem analytically with simplifying assumptions.

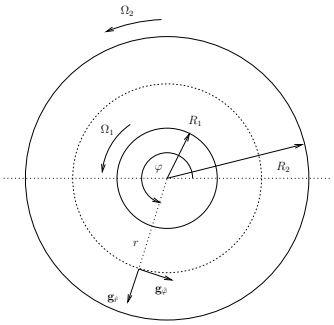



Figure 3.5: Problem geometry.

### 3.4.2 System of governing equations in cylindrical coordinates

Let us consider steady flow. We assume that the velocity field takes the form

$$\mathbf{v} = \mathrm{v}^{\hat{\varphi}}(r)\mathbf{g}_{\hat{\varphi}} = \begin{bmatrix} 0 \\ \mathrm{v}^{\hat{\varphi}}(r) \\ 0 \end{bmatrix}, \tag{3.4.1}$$

then the gradient of $\mathbf{v}$ is given by the formula

$$\nabla\mathbf{v} = \begin{bmatrix} 0 & -\frac{\mathrm{v}^{\hat{\varphi}}}{r} & 0 \\ r\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{\mathrm{v}^{\hat{\varphi}}}{r}\right) + \frac{\mathrm{v}^{\hat{\varphi}}}{r} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \tag{3.4.2}$$

and the symmetric part of the gradient of $\mathbf{v}$ is given by the formula

$$\mathbf{D} = \begin{bmatrix} 0 & \frac{1}{2}r\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{\mathrm{v}^{\hat{\varphi}}}{r}\right) & 0 \\ \frac{1}{2}r\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{\mathrm{v}^{\hat{\varphi}}}{r}\right) & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{3.4.3}$$

Matrices representing $\nabla\mathbf{v}$ and $\mathbf{D}$ are given with respect to the normed basis. Note that it is more convenient to set $\mathrm{v}^{\hat{\varphi}}(r) =_{\mathrm{def}} \omega(r)r$. In such a case the formulae above read

$$\nabla\mathbf{v} = \begin{bmatrix} 0 & -\omega & 0 \\ r\frac{\mathrm{d}\omega}{\mathrm{d}r} + \omega & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{3.4.4}$$

and

$$\mathbf{D} = \begin{bmatrix} 0 & \frac{r}{2}\frac{\mathrm{d}\omega}{\mathrm{d}r} & 0 \\ \frac{r}{2}\frac{\mathrm{d}\omega}{\mathrm{d}r} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{3.4.5}$$

Further

$$[\nabla\mathbf{v}]\,\mathbf{v} = \begin{bmatrix} -r\omega^2 \\ 0 \\ 0 \end{bmatrix} \tag{3.4.6}$$

The temperature field and the pressure field are assumed to be functions of the radial variable $r$,

$$\theta = \theta(r), \tag{3.4.7}$$
$$p = p(r). \tag{3.4.8}$$

The left Cauchy–Green tensor representing the response from the natural to the current configuration is assumed to take the form

$$\mathbf{B}_{\kappa_{p(t)}} = \begin{bmatrix} \mathrm{B}^{\hat{r}}{}_{\hat{r}}(r) & \mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}(r) & 0 \\ \mathrm{B}^{\hat{\varphi}}{}_{\hat{r}}(r) & \mathrm{B}^{\hat{\varphi}}{}_{\hat{\varphi}}(r) & 0 \\ 0 & 0 & \mathrm{B}^{\hat{z}}{}_{\hat{z}}(r) \end{bmatrix}, \tag{3.4.9}$$

where the matrix $\mathbf{A}$ is expressed with respect to the *normed* basis, that is if $\mathbf{B}_{\kappa_{p(t)}} = \mathrm{B}^{\hat{r}}{}_{\hat{r}}(r)\mathbf{g}_{\hat{r}} \otimes \mathbf{g}^{\hat{r}} + \cdots + \mathrm{B}^{\hat{z}}{}_{\hat{z}}(r)\mathbf{g}_{\hat{z}} \otimes \mathbf{g}^{\hat{z}}$, then

$$\operatorname{div} \mathbf{B}_{\kappa_{p(t)}} = \begin{bmatrix} \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\mathrm{B}^{\hat{r}}{}_{\hat{r}}\right) - \frac{\mathrm{B}^{\hat{\varphi}}{}_{\hat{\varphi}}}{r} \\ \frac{\mathrm{dB}^{\hat{\varphi}}{}_{\hat{r}}}{\mathrm{d}r} + \frac{\mathrm{B}^{\hat{\varphi}}{}_{\hat{r}} + \mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}}{r} \\ 0 \end{bmatrix}, \tag{3.4.10}$$

where the vector is expressed with respect to the *normed* basis, that is

$$\operatorname{div} \mathbf{B}_{\kappa_{p(t)}} = \left(\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\mathrm{B}^{\hat{r}}{}_{\hat{r}}\right) - \frac{\mathrm{B}^{\hat{\varphi}}{}_{\hat{\varphi}}}{r}\right)\mathbf{g}_{\hat{r}} + \left(\frac{\mathrm{dB}^{\hat{\varphi}}{}_{\hat{r}}}{\mathrm{d}r} + \frac{\mathrm{B}^{\hat{\varphi}}{}_{\hat{r}} + \mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}}{r}\right)\mathbf{g}_{\hat{\varphi}}. \tag{3.4.11}$$

Further, if $\mathbf{B}_{\kappa_{p(t)}}$ takes the form (3.4.9), then

$$\overset{\triangledown}{\mathbf{B}}_{\kappa_{p(t)}} = \begin{bmatrix} 0 & -r\frac{\mathrm{d}\omega}{\mathrm{d}r}\mathrm{B}^{\hat{r}}{}_{\hat{r}} & 0 \\ -r\frac{\mathrm{d}\omega}{\mathrm{d}r}\mathrm{B}^{\hat{r}}{}_{\hat{r}} & -2r\frac{\mathrm{d}\omega}{\mathrm{d}r}\mathrm{B}^{\hat{\varphi}}{}_{\hat{r}} & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{3.4.12}$$

Consequently, the system of governing equations simplifies to

$$\begin{bmatrix} -\rho r\omega^2 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} -\frac{\mathrm{d}p}{\mathrm{d}r} + \frac{\mathrm{d}}{\mathrm{d}r}\left(G(\theta)\left(\mathrm{B}^{\hat{r}}{}_{\hat{r}} - 1\right)\right) + G(\theta)\frac{\mathrm{B}^{\hat{r}}{}_{\hat{r}} - \mathrm{B}^{\hat{\varphi}}{}_{\hat{\varphi}}}{r} \\ \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^3\mu_2\frac{\mathrm{d}\omega}{\mathrm{d}r} + G(\theta)r^2\mathrm{B}^{\hat{\varphi}}{}_{\hat{r}}\right) \\ 0 \end{bmatrix} \tag{3.4.13a}$$

and

$$\mu_1 \begin{bmatrix} 0 & -r\frac{\mathrm{d}\omega}{\mathrm{d}r}\mathrm{B}^{\hat{r}}{}_{\hat{r}} & 0 \\ r\frac{\mathrm{d}\omega}{\mathrm{d}r}\mathrm{B}^{\hat{r}}{}_{\hat{r}} & -2r\frac{\mathrm{d}\omega}{\mathrm{d}r}\mathrm{B}^{\hat{\varphi}}{}_{\hat{r}} & 0 \\ 0 & 0 & 0 \end{bmatrix} + G(\theta)\begin{bmatrix} \mathrm{B}^{\hat{r}}{}_{\hat{r}} - 1 & \mathrm{B}^{\hat{r}}{}_{\hat{\varphi}} & 0 \\ \mathrm{B}^{\hat{\varphi}}{}_{\hat{r}} & \mathrm{B}^{\hat{\varphi}}{}_{\hat{\varphi}} - 1 & 0 \\ 0 & 0 & \mathrm{B}^{\hat{z}}{}_{\hat{z}} - 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}. \tag{3.4.13b}$$

### 3.4.3 Solution of the steady system

The solution of the transport equation for $\mathbf{B}_{\kappa_{p(t)}}$ (3.4.13b) is the following.

$$\mathrm{B}^{\hat{r}}{}_{\hat{r}} = \mathrm{B}^{\hat{z}}{}_{\hat{z}} = 1, \quad \mathrm{B}^{\hat{r}}{}_{\hat{\varphi}} = \frac{\mu_1}{G(\theta)} r\frac{\mathrm{d}\omega}{\mathrm{d}r}, \quad \mathrm{B}^{\hat{\varphi}}{}_{\hat{\varphi}} = 1 + 2\left(\frac{\mu_1}{G(\theta)} r\frac{\mathrm{d}\omega}{\mathrm{d}r}\right)^2. \tag{3.4.14}$$

After inserting (3.4.14) into (3.4.13a) one gets

$$\frac{\mu_2+\mu_1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^3\frac{\mathrm{d}\omega}{\mathrm{d}r}\right)=0, \tag{3.4.15}$$

which together with the boundary conditions $\omega(R_1)=\Omega_1$ and $\omega(R_2)=\Omega_2$ gives

$$\omega(r)=\frac{R_1^2\Omega_1-R_2^2\Omega_2}{R_1^2-R_2^2}-\frac{R_1^2R_2^2(\Omega_1-\Omega_2)}{r^2(R_1^2-R_2^2)}. \tag{3.4.16}$$

It is worth mentioning that when $G(\theta)$ is the only material parameter depending on $\theta$, the temperature field does not affect the solution of the velocity field. Upon substituting (3.4.16) into (3.4.14) one gets

$$\begin{aligned}
\mathrm{B}^{\hat{r}}{}_{\hat{r}}=\mathrm{B}^{\hat{z}}{}_{\hat{z}}&=1,\\
\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}&=\frac{\mu_1}{G(\theta)}\frac{2R_1^2R_2^2(\Omega_1-\Omega_2)}{r^2(R_1^2-R_2^2)},\\
\mathrm{B}^{\hat{\varphi}}{}_{\hat{\varphi}}&=1+2\left(\frac{\mu_1}{G(\theta)}\frac{2R_1^2R_2^2(\Omega_1-\Omega_2)}{r^2(R_1^2-R_2^2)}\right)^2.
\end{aligned} \tag{3.4.17}$$

Finally, we are interested in the solution for the steady solution for

$$\begin{aligned}
2\mu_2\mathbf{D}_\delta:\mathbf{D}_\delta+\operatorname{div}(\kappa\nabla\theta)+\theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\left(\mathbf{B}_{\kappa_{p(t)}}\right)_\delta:\mathbf{D}_\delta\\
+\frac{1}{2\mu_1}\left(G(\theta)^2-\theta G(\theta)\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)\left(\operatorname{Tr}\mathbf{B}_{\kappa_{p(t)}}+\operatorname{Tr}\left(\mathbf{B}^{-1}_{\kappa_{p(t)}}\right)-6\right)=0.
\end{aligned} \tag{3.4.18}$$

Using Cayley-Hamilton Theorem $\operatorname{Tr}\left(\mathbf{B}^{-1}_{\kappa_{p(t)}}\right)$ can be written as

$$\operatorname{Tr}\left(\mathbf{B}^{-1}_{\kappa_{p(t)}}\right)=\frac{(\operatorname{Tr}\mathbf{B}_{\kappa_{p(t)}})^2-\operatorname{Tr}\left(\mathbf{B}^2_{\kappa_{p(t)}}\right)}{2\det\mathbf{B}_{\kappa_{p(t)}}}. \tag{3.4.19}$$

Since $\mathrm{B}^{\hat{\varphi}}{}_{\hat{\varphi}}=1+2\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}{}^2$ and $\mathrm{B}^{\hat{r}}{}_{\hat{r}}=\mathrm{B}^{\hat{z}}{}_{\hat{z}}=1$, we get

$$\begin{aligned}
\det\mathbf{B}_{\kappa_{p(t)}}&=\mathrm{B}^{\hat{r}}{}_{\hat{r}}\mathrm{B}^{\hat{\varphi}}{}_{\hat{\varphi}}-\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}{}^2=1+\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}{}^2,\\
(\operatorname{Tr}\mathbf{B}_{\kappa_{p(t)}})^2-\operatorname{Tr}\left(\mathbf{B}^2_{\kappa_{p(t)}}\right)&=(3+2\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}{}^2)^2-(2+(1+2\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}{}^2)^2+2\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}{}^2)=\\
&\quad 9+12\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}{}^2+4\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}{}^4-(2+1+4\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}{}^2+4\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}{}^4+2\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}{}^2)=6(1+\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}{}^2).
\end{aligned}$$

Thus,

$$\operatorname{Tr}\left(\mathbf{B}^{-1}_{\kappa_{p(t)}}\right)=\frac{6(1+\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}{}^2)}{2(1+\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}{}^2)}=3. \tag{3.4.20}$$

We will now evaluate all terms in (3.4.18) (note that $\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}=\alpha G(\theta)$)

1.
$$2\mu_2\mathbf{D}_\delta:\mathbf{D}_\delta=\mu_2\left(r\frac{\mathrm{d}\omega}{\mathrm{d}r}\right)^2,$$

2.
$$\operatorname{div}(\kappa\nabla\theta) = \kappa\left(\frac{\mathrm{d}^2\theta}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}\theta}{\mathrm{d}r}\right),$$

3.
$$\theta\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\left(\mathbf{B}_{\kappa_{p(t)}}\right)_\delta : \mathbf{D}_\delta = \theta\alpha G(\theta)\frac{\mu_1}{G(\theta)}\left(r\frac{\mathrm{d}\omega}{\mathrm{d}r}\right)^2 = \theta\alpha\mu_1\left(r\frac{\mathrm{d}\omega}{\mathrm{d}r}\right)^2,$$

4.
$$\frac{1}{2\mu_1}\left(G(\theta)^2 - \theta G(\theta)\frac{\mathrm{d}G(\theta)}{\mathrm{d}\theta}\right)\left(\operatorname{Tr}\mathbf{B}_{\kappa_{p(t)}} + \operatorname{Tr}\left(\mathbf{B}^{-1}_{\kappa_{p(t)}}\right) - 6\right)$$
$$= \frac{G(\theta)^2}{2\mu_1}(1-\theta\alpha)2\left(\frac{\mu_1}{G(\theta)}\right)^2\left(r\frac{\mathrm{d}\omega}{\mathrm{d}r}\right)^2 = \mu_1(1-\theta\alpha)\left(r\frac{\mathrm{d}\omega}{\mathrm{d}r}\right)^2.$$

Summing all together gives

$$(\mu_2+\mu_1)\left(r\frac{\mathrm{d}\omega}{\mathrm{d}r}\right)^2 + \kappa\left(\frac{\mathrm{d}^2\theta}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}\theta}{\mathrm{d}r}\right) = 0. \tag{3.4.21}$$

Upon substituting $\omega$ to (3.4.21) one can find a general solution

$$\theta = C_1 - \frac{C}{4r^2} + C_2\log r, \text{ where } C = \frac{\mu_2+\mu_1}{\kappa}\left(\frac{2R_1^2R_2^2(\Omega_1-\Omega_2)}{R_1^2-R_2^2}\right)^2 \tag{3.4.22}$$

and $C_1, C_2$ have to be determined from the boundary condition.

Let us assume that $\theta(R_1) = \theta_{R_1}$ and $\left.\dfrac{\mathrm{d}\theta}{\mathrm{d}r}\right|_{r=R_2} = 0$, then the solution is

$$\theta = \theta_{R_1} + \frac{C}{4}\left(\frac{1}{R_1^2} - \frac{1}{r^2} - \frac{2}{R_2^2}\log\frac{r}{R_1}\right). \tag{3.4.23}$$

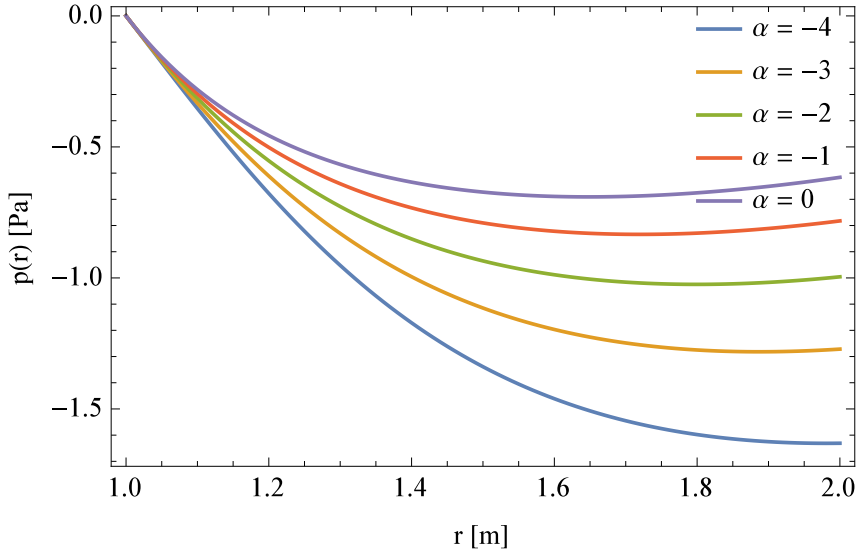
Since $G(\theta)$ is a function of temperature $\theta$ which depends on $r$, $G(\theta)$ is a function of $r$. Finally, the pressure $p(r)$ is obtained from (3.4.13a)

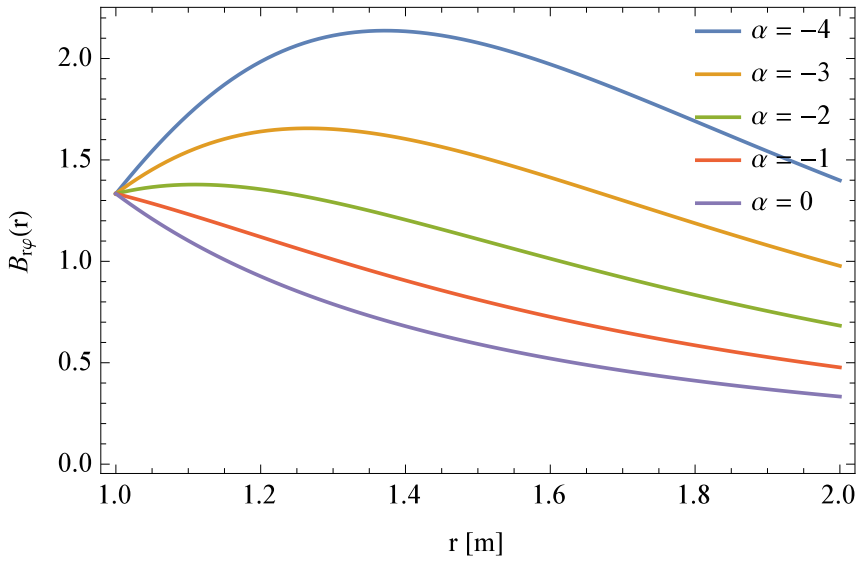
$$\frac{\mathrm{d}p}{\mathrm{d}r} = \rho\omega^2 r - 2r\frac{\mu_1^2}{G(\theta)}\left(\frac{\mathrm{d}\omega}{\mathrm{d}r}\right)^2 \tag{3.4.24}$$

by numerical integration. Note that only a gradient of the pressure $p$ is present in the balance of linear momentum and thus its value is known only up to the constant $C$. This constant is fixed by imposing the boundary condition $p(r = R_1) = 0$ giving

$$p(r) = \int_{R_1}^{r}\rho\omega^2(s)s - 2s\frac{\mu_1^2}{G(\theta(s))}\left(\frac{\mathrm{d}\omega(s)}{\mathrm{d}s}\right)^2\mathrm{d}s. \tag{3.4.25}$$

Temperature dependence of the model is driven by the factor $\alpha$. For $\alpha = 0$ we obtain a standard set of material coefficients without any influence of temperature. We demonstrate the dependence of the model on temperature by plotting analytical results for $\alpha \in \{0, -1, -2, -3, -4\}$ shown in Figure 3.6.



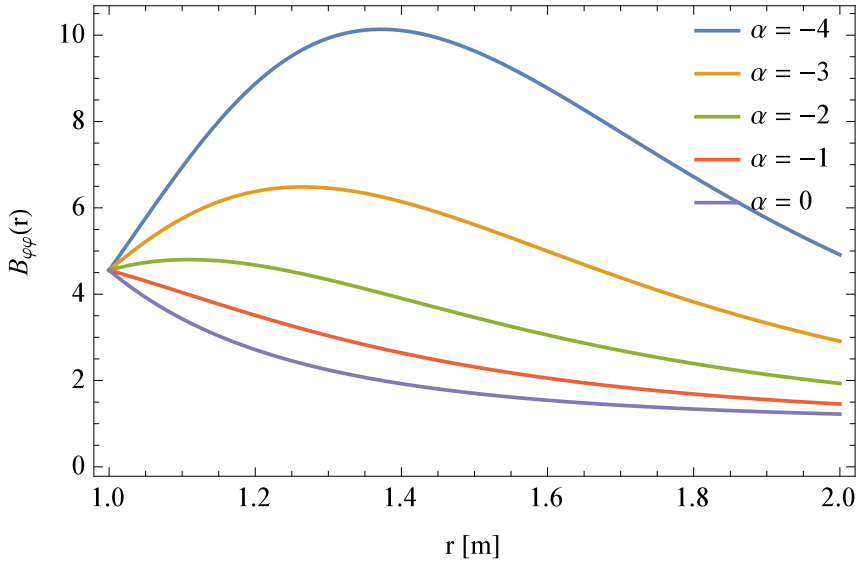




Figure 3.6: The influence of the temperature for different $\alpha$ on quantities $p(r)$, $\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}(r)$ and $\mathrm{B}^{\hat{\varphi}}{}_{\hat{\varphi}}(r)$, respectively. Other quantities $\omega(r)$, $\mathrm{B}^{\hat{r}}{}_{\hat{r}}(r)$ and $\theta$ are not influenced by the factor $\alpha$.

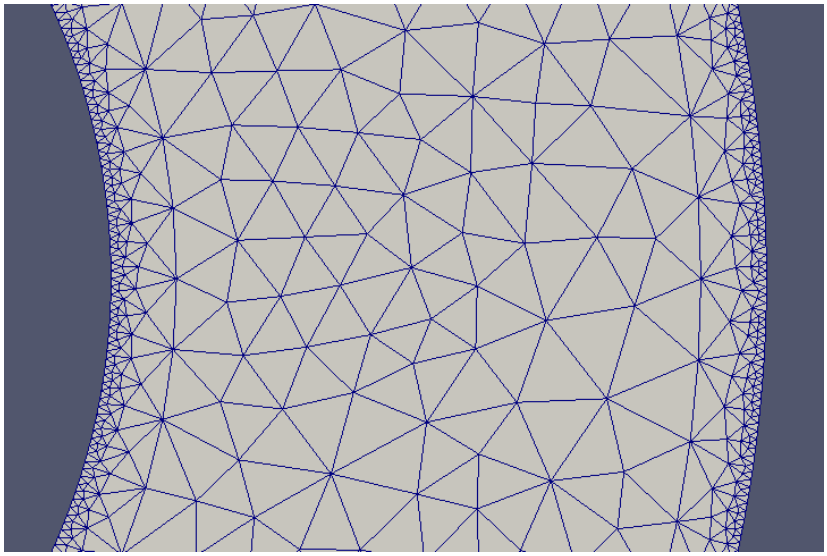


Figure 3.7: A part of the computational mesh for cylinder Couette flow.

### 3.4.4 Simulation results

We have found a semi-analytic solution of the full 3D problem, but we can get the same formulas for a semi-analytic solution if we consider the problem to be only 2D (as depicted in Figure 3.5). Therefore we can compare analytic results with results of simulation in 2D.

For the simulation we use the weak formulated model T-Oldroyd-B described in 3.1.3 with material coefficients

$$\rho = \mu_1 = \mu_2 = \kappa = c_V = 1, \quad G(\theta) = G_0 e^{\alpha(\theta-\theta_R)}$$

for

$$G_0 = 1, \quad \alpha = -0.1, \quad \theta_R = 273.$$

Angular velocities of the fluid are $\Omega 1 = 0$ and $\Omega 2 = 0.5$ for radii $R_1 = 1$, $R_2 = 2$, respectively. We also fixed pressure $p(R_1) = 0$ and $\theta(R_1) = \theta_R$ on the inner cylinder. The computation is done in the Cartesian coordinates, the computational mesh consists of 9520 elements which are refined near the boundaries, and part of the mesh is depicted in Figure 3.7.

To compare FEM results with analytic ones we plot the quantities $\mathrm{v}^{\hat{\varphi}}(r) = r\omega(r)$, $p(r)$, $\theta$, $\mathrm{B}^{\hat{r}}{}_{\hat{r}}(r)$, $\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}(r)$, $\mathrm{B}^{\hat{\varphi}}{}_{\hat{\varphi}}(r)$ in graph 3.8. The FEM results and analytical are identical up to discretization error therefore we can conclude that our implementation is all right.

## 3.5 Small Amplitude Oscillations

In this chapter, we only sketch our recent work. In the first chapter, small amplitude oscillations constants were introduced for models consisting of mechanical analogues. The oscillatory experiment is now performed with a rectangular piece of material for model T-Maxwell-B and we want to compare the results with the 1D oscillations constant $G^*$.

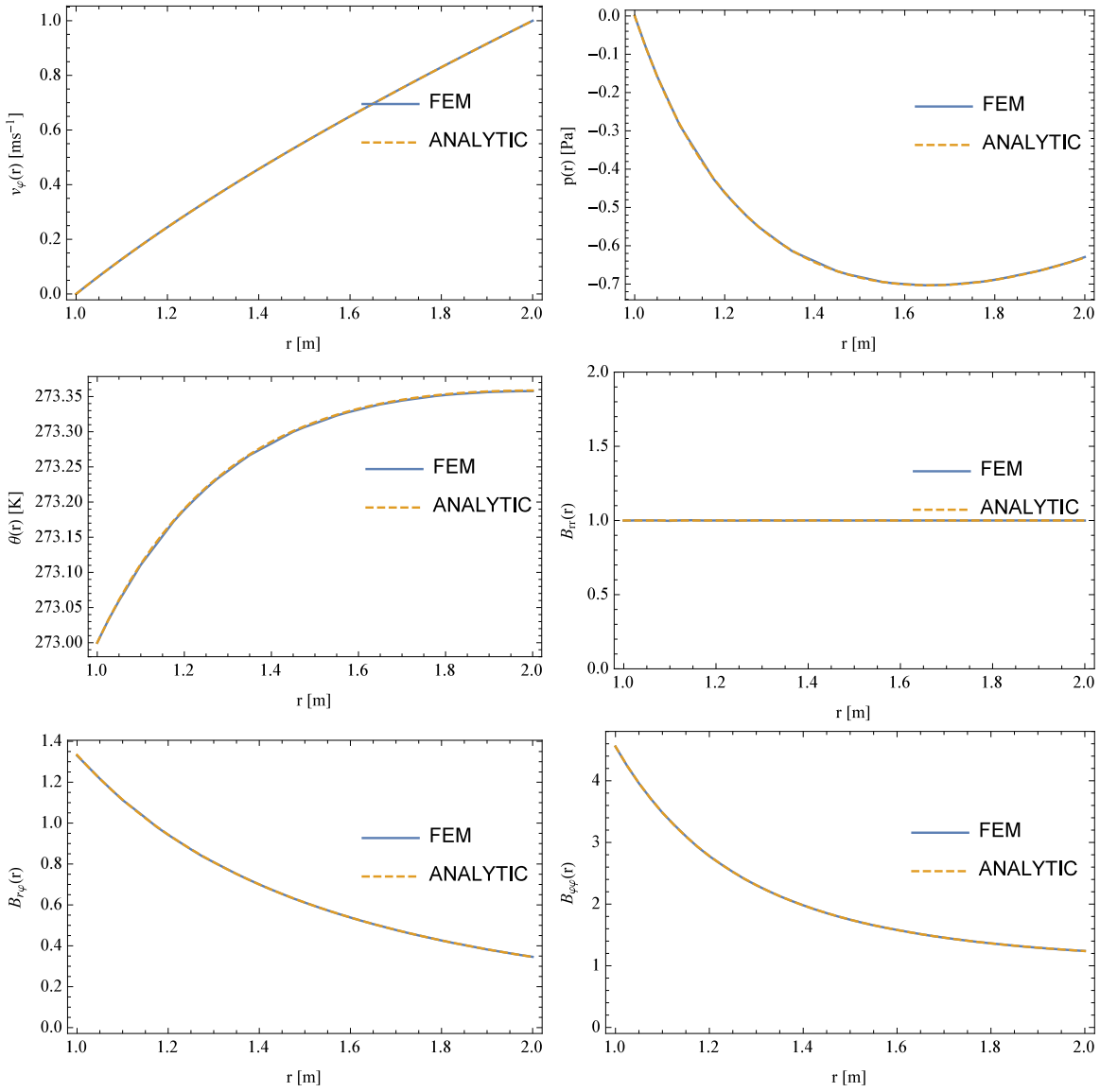



Figure 3.8: Comparison of analytic and FEM results of $\mathrm{v}^{\hat{\varphi}}(r)$, $p(r)$, $\theta$, $\mathrm{B}^{\hat{r}}{}_{\hat{r}}(r)$, $\mathrm{B}^{\hat{r}}{}_{\hat{\varphi}}(r)$ and $\mathrm{B}^{\hat{\varphi}}{}_{\hat{\varphi}}(r)$, respectively.

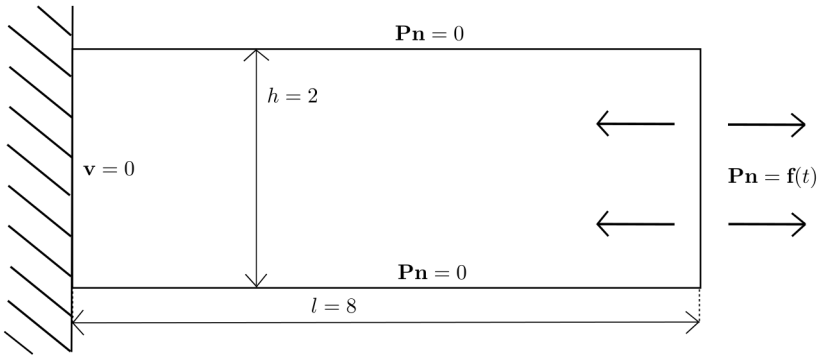



Figure 3.9: Geometry and boundary conditions of the oscillatory problem.

### 3.5.1 Problem Description

The goal is to perform sinusoidal oscillation on a rectangular piece of material and to capture the response. We prescribe the normal stress $\sigma := \mathbf{Pn}$ and observe the strain response $\epsilon$. A geometry of a experiment is very similar to the benchmark problem for ALE method and is depicted on (3.9). *Do nothing* $\mathbf{Pn} = 0$ boundary conditions are prescribed on the top and bottom of the rectangular of length $l = 8$ and hight $h = 2$. Left side carries the *no slip* boundary condition $\mathbf{v} = 0$. Right side $\Gamma_R$ is forced to oscillate by the condition $\mathbf{Pn} = \mathbf{f}(t)$, where $\mathbf{f}(t) = (\sin \omega t, 0)$ for some frequency $\omega \in \mathbb{R}$.

# Conclusion

Derivation of temperature dependent models was successful in the case of the thermodynamic system consisting of springs and dashpots, but also in the case of a real material, which was the main part. We have shown that the framework proposed by Rajagopal and Srinivasa can be extended by the temperature influence and we obtain thermodynamic compatible models T-Oldroyd-B, T-Maxwell and T-Quad1 which indeed reduces to the models Oldroyd-B, Maxwell and Quad1 presented in [15] thesis. Let us note that the general evolution equation for the temperature (2.1.13) evaluated for neo-Hookean free energy is identical to the temperature evolution arising from mechanical analogues (1.2.7) (if we identify $\epsilon^{el} = \mathbf{B}_{\kappa_p(t)}$). Hence the full T-Maxwell model and the 1D one are very similar in some sense.

We have found out that if we consider a standard geometry for Maxwell element (in terms of mechanical analogues) and consider temperature dependent material coefficients, we obtain the T-Maxwell model

$$\dot{\epsilon} = \frac{\sigma}{\nu(\theta)} + \frac{\dot{\sigma}}{k(\theta)} - \dot{\theta}\frac{\sigma k'(\theta)}{k^2(\theta)}, \tag{3.5.1}$$

$$c_V\dot{\theta} = \frac{\sigma^2}{\nu(\theta)} - (k(\theta) - \theta k'(\theta))\frac{\sigma}{k(\theta)}\left(\dot{\epsilon} - \frac{\sigma}{\nu(\theta)}\right) + r \tag{3.5.2}$$

with one extra term in a constitutive equation in comparison with the standard one.

During the simulations with mechanical analogues, we observed a cooling of the system due to increasing strain. One would intuitively say the opposite, although , at the end, it makes sense and agrees with a real experiment on an elastic rubber when stretched. It also reveals the meaning of the term with the second derivation of free energy in the evolution equation of temperature. And this is one reason, why analogy with simple systems is important - this phenomenon is not very strong for real materials, since real materials always exhibit some dissipation.

In the third chapter, weak formulated models were implemented and verified. The first benchmark was the a classical flow past cylinder benchmark for Oldroyd-B. Then we develop analytical solution for a uni-axial stretching of a rectangular piece of neo-Hookean material to verify the implementation of ALE method. Further we tested the full temperature model T-Oldroyd-B on the steady problem of Couette flow between two cylinders and compare it with analytical solution.

Recently we are working on the comparison of small amplitude oscillations in 2D with the oscillation constant $G^*$. Aim is to find out, how big is the error in fit due to the 2D geometry. We are also work on the oscillatory experiment of the piece of glass. We want to melt it by its own production of heat due to the oscillations.

# Bibliography


[1] Utkarsh Ayachit. *The ParaView Guide: A Parallel Visualization Application*. Kitware, Inc., USA, 2015.

[2] S.S. Bhavikatti. *Finite Element Analysis*. New Age International, 2005.

[3] Miroslav Bulíček, Eduard Feireisl, and Josef Málek. A navier–stokes–fourier system for incompressible fluids with temperature dependent material coefficients. *Nonlinear Analysis: Real World Applications*, 10(2):992–1015, 2009.

[4] H.B. Callen. *Thermodynamics and an Introduction to Thermostatistics*. Wiley, 1985.

[5] Jean Donea, Antonio Huerta, J.-Ph. Ponthot, and A. Rodríguez-Ferran. *Arbitrary Lagrangian–Eulerian Methods*. John Wiley and Sons, Ltd, 2004.

[6] A. D. Drozdov. Effect of temperature on the viscoelastic and viscoplastic behavior of polypropylene. *Mechanics of Time-Dependent Materials*, 14(4):411–434, 2010.

[7] Christophe Geuzaine and Jean-François Remacle. Gmsh: a three-dimensional finite element mesh generator with built-in pre- and post-processing facilities. *International Journal for Numerical Methods in Engineering*, 79(11):1309–1331, 2009.

[8] Martien A. Hulsen, Raanan Fattal, and Raz Kupferman. Flow of viscoelastic fluids past a cylinder at high weissenberg number: Stabilized simulations using matrix logarithms. *Journal of Non-Newtonian Fluid Mechanics*, 127(1):27 – 39, 2005.

[9] Kolumban Hutter and 1960 Jöhnk, Klaus. *Continuum Methods of Physical Modeling : Continuum Mechanics, Dimensional Analysis, Turbulence*. Berlin New York Springer, 2004. Includes bibliographical references (pages 603-614) and indexes.

[10] A. Logg, K.A. Mardal, and G. Wells. *Automated Solution of Differential Equations by the Finite Element Method: The FEniCS Book*. Lecture Notes in Computational Science and Engineering. Springer Berlin Heidelberg, 2012.

[11] K.P. Menard. *Dynamic Mechanical Analysis: A Practical Introduction, Second Edition*. CRC Press, 2008.

[12] K. R. Rajagopal and A. R. Srinivasa. A thermodynamic frame work for rate type fluid models. *Journal of Non-newtonian Fluid Mechanics*, 88:207–227, 2000.

[13] K. R. Rajagopal and A. R. Srinivasa. On the thermomechanics of materials that have multiple natural configurations part i: Viscoelasticity and classical plasticity. *Zeitschrift für angewandte Mathematik und Physik ZAMP*, 55(5):861–893, 2004.

[14] K. R. Rajagopal and A. R. Srinivasa. On thermomechanical restrictions of continua. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 460(2042):631–651, 2004.

[15] Karel Tůma. *Identification of rate type fluids suitable for modeling geomaterials*. PhD thesis, Mathematical Institute, Charles University, 2013.

[16] A.S. Wineman and K.R. Rajagopal. *Mechanical Response of Polymers: An Introduction*. Cambridge University Press, 2000.

[17] R.K. Zeytounian. *Navier-Stokes-Fourier Equations: A Rational Asymptotic Modelling Point of View*. Springer Berlin Heidelberg, 2012.