Analysis of Non-Newtonian and Two-Phase Flows

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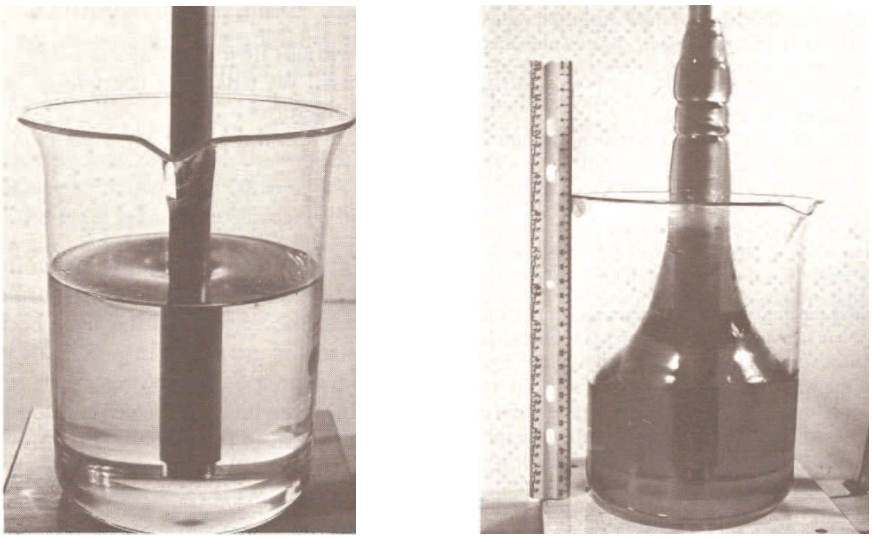
Chapter 1

Introduction

Fluids can be classified according to various criteria. One opportunity is to distinguish *Newtonian* and *non-Newtonian* fluids. The difference between both classes of fluids can be observed in a variety of situations. For example, consider two bowls containing two different types fluids, e.g., water and a polymer solution representing a Newtonian and a non-Newtonian fluid, respectively. Inserting a rotating rod in each bowl (see figure 1.1), we observe that in case of the Newtonian fluid, a characteristic dip arises near the rotating rod due to centrifugal forces pushing the fluid outwards. In contrast, some non-Newtonian fluids climb up along the rod. This effect is known as the *Weissenberg effect* [BAH77], [Tan88].



(a) Newtonian (b) Non-Newtonian

Figure 1.1: Weissenberg Rod Climbing Effect [BAH77].

Particularly, in industrial applications non-Newtonian fluids are of great interest, since many used fluids, e.g., lacquers or polymer solutions show non-Newtonian effects.

In general, real-world experiments of industrial processes can be complex, cost-intensive, and time-consuming. Therefore, numerical simulations are important and can be useful in order to optimize the process with respect to cost or quality aspects. Thus, the investigation of mathematical models governing the flow of non-Newtonian fluids is important regarding both analysis and numerical simulations. In the context of this thesis, the term analysis in the title refers to both the meaning in the mathematical sense and the more informal meaning of "computational analysis", i.e., the numerical investigation of the behavior of non-Newtonian fluids.

Non-Newtonian fluids are characterized by different features, such as viscosity, elasticity, or memory effects. An important feature of polymeric liquids is the fact that their viscosity changes with the shear rate, so-called *generalized Newtonian fluids* on which this thesis is focused on. The mathematical model describing the motion of these fluids is given by the system

$$\begin{aligned} \tfrac{\partial}{\partial t}\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} &= \operatorname{div}\mathbf{S} - \nabla p + \mathbf{f}, && \text{on } [0,T]\times\mathbb{R}^n \\ \operatorname{div}\mathbf{u} &= 0, && \text{on } [0,T]\times\mathbb{R}^n \\ \mathbf{u}_{|_{t=0}} &= \mathbf{u}_0, && \text{on } \mathbb{R}^n. \end{aligned} \tag{1.1}$$

Here, the stress tensor $\mathbf{S}$ is given by $\mathbf{S} = 2\,\mu(\|\mathbf{D}\|^2)\mathbf{D}$ with the rate-of-deformation tensor $\mathbf{D} = \frac{1}{2}\left[\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right]$, and the viscosity function μ depending on $\|\mathbf{D}\|^2$ respectively on the shear rate $\dot{\gamma} = \sqrt{2}\,\|\mathbf{D}\|$, where $\|\mathbf{D}\|$ denotes the Hilbert-Schmidt norm.

The main result of this thesis is the proof of existence of problem (1.1) in the maximal L_p-regularity class. By means of maximal L_p-regularity, local (in time) strong well-posedness of this model is obtained under certain restrictions concerning the viscosity function. For example, for the viscosity function

$$\mu(\|\mathbf{D}\|^2) = \mu_0(1 + \|\mathbf{D}\|^2)^{\frac{m-2}{2}}$$

with $\mu_0 > 0$ which is often used in the mathematical literature, we obtain local existence in $\mathbb{R}^n, (n > 1)$ for $m > \frac{3n-4}{2(n-1)}$, i.e., in the 3D case $m > 5/4$ is sufficient. We emphasize that according to the engineering literature the range of interest concerning m is $m > 1$.

In the numerical part, the emphasis is on two-phase flows, since many interesting problems appear in this context. Moreover, we compare experiment and simulation of a binary droplet collision using non-Newtonian fluids, the behavior of which is assumed to be that of generalized Newtonian fluids. Furthermore, assuming the situation of system (1.1), we show the admissibility of the viscosity function used in the simulation.

The remainder of the thesis is organized as follows. Starting from the physical science with some general notations and introducing the meaning of non-Newtonian fluids, we obtain an insight into the variety and the modeling of non-Newtonian fluids. The main subject of chapter 2 is the development of constitutive equations, i.e., of relations between the velocity field $\mathbf{u}$ and the stress tensor $\mathbf{S}$ which depend on the used substance. The simplest constitutive equation for an incompressible viscous Newtonian fluid

is given by the linear relation $\mathbf{S} = 2\mu\mathbf{D}$ with the constant dynamical viscosity μ and the rate-of-deformation tensor $\mathbf{D}$. Among others, we find out the constitutive equations for describing the Weissenberg effect (see figure 1.1). In particular, we obtain the constitutive equations for generalized Newtonian fluids, which result from the linear relation for incompressible viscous Newtonian fluids by replacing the constant viscosity μ by a function depending on the shear rate $\dot{\gamma}$.

In chapter 3, we concentrate on generalized Newtonian fluids and develop the proof of existence and uniqueness of local (in time) strong solutions of problem (1.1) by means of maximal L_p-regularity. The main result is stated in theorem 3.3.1. We close this chapter with a survey about some results given in mathematical literature and compare our existence result.

Chapter 4 completes the expositions about non-Newtonian fluids with a look at the numerical modeling of two-phase flow. We start with some fundamental concepts solving the Navier-Stokes system numerically, such as the time-splitting method of Chorin [Cho68] and the finite volume method, e.g., [FP02]. Then, we discuss the physical features of two-phase flow modeling, in particular the treatment of the interface. For the description of the interface we employ the volume of fluid (VOF) method and discuss different methods to take the surface tension into account. In this context, we also study spurious currents. Finally, this chapter is complemented with the comparison of experiment and simulation of a binary droplet collision using a particular non-Newtonian fluid. The behavior of this fluid can be assumed to be that of a generalized Newtonian fluid. For the viscosity function used in the simulation, we show that a local strong solution for system (1.1) does exist. Of course, this result is only valid for one-phase flows in the full space $\mathbb{R}^n$. We close this chapter with an existence result of Escher, Prüss, and Simonett [EPS03] for two-phase flows of Newtonian fluids.

Chapter 2

Mathematical Modeling of Non-Newtonian Fluids

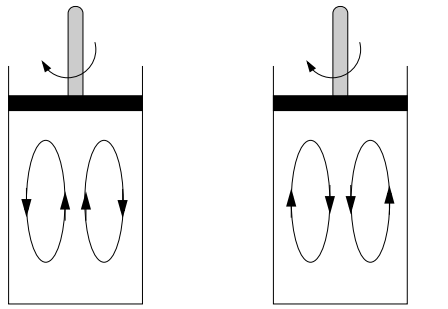
In this chapter, mathematical models governing the flow in particular of non-Newtonian fluids will be studied. Several experiments are recalled, which show the differences in the behavior of Newtonian and non-Newtonian fluids. The notions of *viscosity*, *shear rate*, and *normal stress differences* are introduced and the definition of a generalized Newtonian fluid is explained. In particular, the experiment of the so-called *steady simple shear flow* is described which appears frequently throughout this chapter. Additionally, a short overview is given on how constitutive equations are obtained. Different approaches are described together with their relations.

2.1 Motivation

In order to predict the behavior of particular flows, one needs to take into account the specific type of fluid to be investigated. If two different types of fluids are exposed the same physical situation, it is possible to observe completely different flow behavior, as already observed in the example of the Weissenberg effect (see figure 1.1).

Another interesting experiment is sketched in figure 2.1. There are two bowls containing two different types of fluids, e.g., water and a polymer solution. In the following, we distinguish these fluids with the general notion of Newtonian[1] fluid (for water) and a non-Newtonian[1] fluid (for the polymer solution). Here, the flow is generated by placing a rotating lid on top of the bowls. Assuming the Reynolds number of this flow is large enough, a primary flow for both fluids emerges in the tangential direction and two different secondary flows are produced. For Newtonian fluids, there are no forces to counter the centrifugal force. Therefore, a secondary flow is produced which is directed radially outwards close to the lid and a vortex as shown in figure 2.1(a) arises. Instead, the secondary flow of the non-Newtonian fluid generates a vortex in the opposite direction to the experiment with the Newtonian fluid [BAH77] as depicted in figure 2.1(b).

[1] For the distinction of Newtonian and non-Newtonian fluids see definition 2.5.3.



(a) Newtonian (b) Non-Newtonian

Figure 2.1: Secondary Flow in Rotating Lid System.

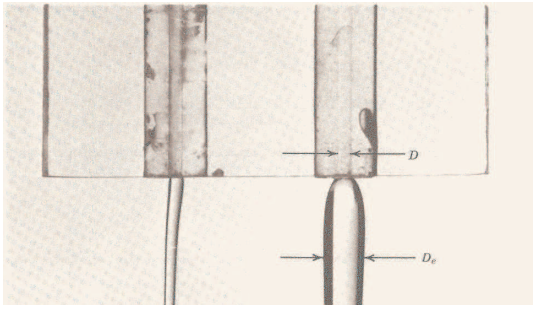


Figure 2.2: Extrudate Swell [BAH77]. *(left)* Newtonian. *(right)* Non-Newtonian.

Next, we consider an experiment which is more difficult to analyze, than the experiments of the Weissenberg effect and the rotating lid system. For the latter we will obtain an idea of their constitutive equations at the end of this chapter. In figure 2.2, there are two tubes: one is filled up with a Newtonian and the other one with a non-Newtonian fluid. At the bottom of each tube is a circular hole with the diameter D. A stream of a Newtonian fluid shows no significant diameter increase (see figure 2.2*(left)*) in contrast to a non-Newtonian fluid where the diameter of the extrudate is found to be larger than the hole diameter (see figure 2.2*(right)*). With some polymers extrudate diameters can reach up to three or four times of the hole diameter [BAH77]. An experiment concerning the viscosity effect, is given at the end of chapter 4.

In general, several effects can occur, such as viscosity, elasticity or memory effects. If the fluid shows pure elasticity effects, this means that it "remembers" its state of balance and tries to redress its balance state. For example, a spring returns to its original state when its steering force disappears. A pure elastic fluid does not "remember" its deformation history, whereas fluids with memory depend on their deformation history, i.e., they "remember" not only their original state. For more details see, e.g., [BAH77], [Gie94].

Before interpreting some of these aspects in more detail and showing how the different effects are taken into account, we have a closer look at the balance equations.

2.2 Notation

In the following, let n be the space dimension, usually $n = 3$, let $\Omega \subset \mathbb{R}^n$ be a domain with $\partial\Omega \in C^1$, and $J \subset \mathbb{R}_+$ a time interval. Then $(t, \mathbf{x}) \in J \times \Omega$ denotes the position $\mathbf{x}$ at time t. The velocity of a flow field is given by $\mathbf{u} = \mathbf{u}(t, \mathbf{x})$. If reasonable, the dependencies of t and $\mathbf{x}$ are neglected to achieve a better legibility. $\nabla\mathbf{u} = \nabla_x\mathbf{u} = (\partial u_1/\partial x_1, \ldots, \partial u_n/\partial x_n)^T$ is the gradient of $\mathbf{u}$ with respect to the spatial variables. Vectors and tensors are written in bold face and their components are denoted by $i = 1, \ldots, n$

and $i, j = 1, \ldots, n$, respectively. For example, $\mathbf{x} = (x_1, \ldots, x_n)^T \in \mathbb{R}^n$ and $\mathbf{T} = (T_{ij})_{i,j=1,\ldots,n} \in \mathbb{R}^{n\times n}$, respectively. The unit matrix is given by $\mathbf{I} \in \mathbb{R}^{n\times n}$, and $\mathbf{e}_i$ denotes the i^{th} unit base vector of the absolute cartesian reference frame with $i = 1, \ldots, n$. The divergence $(\nabla\cdot)$ of a matrix is defined as $\nabla\cdot\mathbf{T} = (\nabla\cdot(\mathbf{T}_{1j})_{j=1,\ldots,n}, \ldots, \nabla\cdot(\mathbf{T}_{nj})_{j=1,\ldots,n})^T$. The surface and volume measures are expressed by dA and $d\mathbf{x}$. Concerning the modeling, flow fields are supposed to be as smooth as necessary such that all needed quantities are well-defined.

Consider a fluid flow in a domain $\Omega \subset \mathbb{R}^n$. The motion of the fluid is characterized by the following variables: the velocity $\mathbf{u} : J \times \Omega \to \mathbb{R}^n$, the pressure $p : J \times \Omega \to \mathbb{R}$ and the density $\rho : J \times \Omega \to \mathbb{R}$. If the velocity is independent of time, the flow is called *steady*, otherwise *unsteady*.

Two possibilities for the description of flows are common, either using a reference frame moving with the fluid, known as *Lagrange description*, or using a fixed reference frame, known as *Euler* or *field description*, respectively. The Lagrange description means to consider a given quantity of matter moving with the fluid. An observer situated on a moving particle sees the changes in velocity, pressure, and density at each position. In fact, a fluid particle is selected and is pursued on its onwards course. Thus, each particle is assigned to an initial position $\mathbf{x}_0$ at time $t = t_0$. The instantaneous position of this particle is then described by the particle path $\Phi(t) := \Phi(t; t_0, \mathbf{x}_0)$. The independent variables of a physical quantity ψ are the time t and the position $\Phi(t)$ of the particle in space which is called *material* or *substantial coordinate*. Thus, the velocity of the particle is given by $\frac{\partial}{\partial t}\Phi(t) = \mathbf{u}(t, \Phi(t))$, i.e., $\Phi(t; t_0, \mathbf{x}_0)$ is the solution of

$$\frac{\partial}{\partial t}\Phi(t) = \mathbf{u}(t, \Phi(t)), \qquad \Phi(t_0) = \mathbf{x}_0.$$

From the physical point of view, the Lagrange description is preferred since the conservation laws are more natural in this description. Studying the dynamics of solid bodies, the identification of the substantial volume is apparent in contrast to studying the dynamics of fluids. Thus, for the study of fluids the Euler description is preferred. Here, an observer positioned at location $\mathbf{x}$ studies the changes which take place in velocity, pressure, and density as the fluid passes through this point. The independent variables of a physical quantity ψ are the time t and the position $\mathbf{x} \in \Omega$ which is denoted as *spatial coordinate*.

Taking a function $\psi(t, \mathbf{x}) = \psi(t, \Phi)$ expressed in spatial or material coordinates, two different time derivatives can be formulated,

$$\begin{aligned} \frac{d}{dt}\psi(t, \mathbf{x}) &= \frac{\partial}{\partial t}\psi(t, \mathbf{x}) \qquad \text{and} \\ \frac{d}{dt}\psi(t, \Phi(t)) &= \frac{\partial}{\partial t}\psi(t, \Phi) + \nabla\psi(t, \Phi)\cdot\frac{\partial}{\partial t}\Phi \\ &= \frac{\partial}{\partial t}\psi(t, \Phi) + \nabla\psi(t, \Phi)\cdot\mathbf{u}(t, \Phi). \end{aligned} \tag{2.1}$$

The derivative along $\Phi(t)$, equation (2.1), is called *Lagrange derivative* or *substantial*

derivative and is denoted by D/Dt. Hence,

$$\frac{D}{Dt}\psi = \frac{\partial}{\partial t}\psi + \mathbf{u} \cdot \nabla\psi. \tag{2.2}$$

The first term of the right-hand side of equation (2.2) describes the local change, whereas the second term states the convective change.

Let Ψ be any extensive quantity, i.e., dependent on the quantity of material of the considered system such as mass and momentum. Then, let ψ be its corresponding intensive quantity, i.e., independent of the quantity of the material of the considered system such as density (mass per unit volume) and velocity (momentum per mass). Furthermore, for $B_0 \subset \Omega$ compact with $\partial B_0 \in C^1$ let $B(t) = \{\Phi(t; t_0, \mathbf{x}_0) : \mathbf{x}_0 \in B_0\}$. Then, the extensive quantity Ψ in the substantial volume $B(t)$ can be expressed by

$$\Psi(t) = \int_{B(t)} \psi(t, \mathbf{x})\, d\mathbf{x}.$$

In order to balance the extensive quantity Ψ in material coordinates, we state Reynolds transport theorem.

Theorem 2.2.1 (Reynolds Transport Theorem) *Let $\mathbf{u} \in C^1(J \times \Omega; \mathbb{R}^n)$ be bounded. For each $(t_0, \mathbf{x}_0) \in J \times \Omega$ is $\Phi(t; t_0, \mathbf{x}_0)$ solution of*

$$\frac{\partial}{\partial t}\Phi(t) = \mathbf{u}(t, \Phi(t)), \qquad \Phi(t_0) = \mathbf{x}_0. \tag{2.3}$$

For $B_0 \subset \Omega$ compact and $\partial B_0 \in C^1$ let

$$B(t) = \{\Phi(t; t_0, \mathbf{x}_0) : \mathbf{x}_0 \in B_0\}$$

be the volume moving with the velocity $\mathbf{u}$. Let $\psi \in C^1(J \times \mathbb{R}^n)$. Then

$$\frac{d}{dt}\int_{B(t)} \psi(t, \mathbf{x})\, d\mathbf{x} = \int_{B(t)} \frac{\partial}{\partial t}\psi(t, \mathbf{x})\, d\mathbf{x} + \int_{\partial B(t)} \psi(t, \mathbf{x})\mathbf{u}(t, \mathbf{x}) \cdot \mathbf{n}(t, \mathbf{x})\, dA, \tag{2.4}$$

where $\mathbf{n}$ denotes the outer normal on ∂B.

A proof can be found, e.g., in [CM79], [Ser59].

In case of an incompressible[2] fluid (the velocity field $\mathbf{u}$ is divergence free) and with $\psi(t, \mathbf{x}) = \rho(t, \mathbf{x})\phi(t, \mathbf{x})$, equation (2.4) can be written as

$$\frac{d}{dt}\int_{B(t)} \rho(t, \mathbf{x})\phi(t, \mathbf{x})\, d\mathbf{x} = \int_{B(t)} \rho(t, \mathbf{x})\frac{D}{Dt}\phi(t, \mathbf{x})\, d\mathbf{x},$$

with the operator D/Dt from equation (2.2).

[2] See definition 2.3.1.

Examining the material volume $B(t)$ at an instant time t, then we can consider that it coincide with a fixed volume B. Therefore, equation (2.4) can be written as

$$\frac{d}{dt}\int_{B(t)} \psi(t,\mathbf{x})\, d\mathbf{x} = \frac{\partial}{\partial t}\int_B \psi(t,\mathbf{x})\, d\mathbf{x} + \int_{\partial B} \psi(t,\mathbf{x})\mathbf{u}(t,\mathbf{x})\cdot\mathbf{n}(t,\mathbf{x})\, dA. \tag{2.5}$$

Then, the first term on the right-hand side of equation (2.5) can be interpreted as the change of Ψ in the fixed volume B and the second term describes the in- and outflow across the boundary ∂B. Hence, the quantity $\psi\mathbf{u}$ denotes the *convective flux* of the quantity Ψ. Then, the balance equation for Ψ in spatial coordinates is always of the form

$$\begin{array}{c}\text{Time rate of}\\ \text{change of } \Psi \text{ in } B\end{array} = \begin{array}{c}-\ \text{Flux of } \Psi\\ \text{across } \partial B \text{ to}\\ \text{the outside}\end{array} + \begin{array}{c}\text{Rate of } \Psi \text{ due to}\\ \text{sources}\end{array} - \begin{array}{c}\text{Rate of } \Psi \text{ due to}\\ \text{sinks}\end{array}$$

see [BSL02], [CM79].

Let $\mathbf{q} : J\times\Omega \to \mathbb{R}^n$ be the flux of Ψ, ∂B the boundary of B with its outer unit normal $\mathbf{n}$, and $f : J\times\Omega \to \mathbb{R}$ represent the intensity of the sources and sinks, respectively. Then, the balance equation of the quantity Ψ is given as follows

$$\frac{d}{dt}\int_B \psi(t,\mathbf{x})\, d\mathbf{x} = -\int_{\partial B} \mathbf{q}(t,\mathbf{x})\cdot\mathbf{n}\, dA + \int_B f(t,\mathbf{x})\, d\mathbf{x}.$$

If $\Psi \in C^1(J\times\Omega), \mathbf{q} \in C^1(J\times\Omega;\mathbb{R}^n)$ and $f \in C(J\times\Omega)$, the application of the divergence theorem of Gauss yields

$$\int_B \left(\frac{\partial}{\partial t}\psi(t,\mathbf{x}) + \nabla\cdot\mathbf{q}(t,\mathbf{x}) - f(t,\mathbf{x})\right) d\mathbf{x} = 0, \qquad \forall\, B\subset\Omega,\ \partial B \in C^1. \tag{2.6}$$

Choosing $B = B_r(\mathbf{x})$, the division by its volume $|B_r(\mathbf{x})|$ and $r \to 0+$ leads to the local balance equation

$$\frac{\partial}{\partial t}\psi(t,\mathbf{x}) + \nabla\cdot\mathbf{q}(t,\mathbf{x}) = f(t,\mathbf{x}), \quad \text{for } t\in J, \mathbf{x}\in\Omega, \tag{2.7}$$

since equation (2.6) is valid for all $B\subset\Omega$ with $\partial B \in C^1$.

For geometrical volumes moving with a constant velocity, we recall the Leibniz rule [Sla99] which will be used in chapter 4.

Theorem 2.2.2 (Leibniz Rule) *Let $B(t)$ be a time dependent region with $\partial\Omega \in C^1$ and let $\psi \in C^1(J\times\Omega)$. Then*

$$\frac{d}{dt}\int_{B(t)} \psi(t,\mathbf{x})\, d\mathbf{x} = \int_{B(t)} \frac{\partial}{\partial t}\psi(t,\mathbf{x})\, d\mathbf{x} + \int_{\partial B(t)} \psi\mathbf{u}_S\cdot\mathbf{n}\, dA,$$

where $\mathbf{u}_S$ denotes the velocity of the boundary ∂B and $\mathbf{n}$ the outer normal on ∂B.

In the case that the geometrical volume just moves with the particle velocity $\mathbf{u}$ (from theorem 2.2.1), i.e., $\mathbf{u}_S = \mathbf{u}$, the volume is no longer arbitrary – instead the volume coincides with the substantial volume. Thus, we obtain Reynolds transport theorem (2.2.1) as a specialization of the Leibniz rule (2.2.2).

2.3 Balance Equations

From the physical point of view it is natural to consider the conservation laws for an extensive quantity in substantial coordinates. Then, in order to deal with the flow within a certain spatial region, the conservation laws will be transformed to spatial coordinates via Reynolds transport theorem.

The total mass $m : J \to \mathbb{R}$ of the fluid inside a substantial domain $B(t) \subset \Omega(t)$ at a fixed time t is given by

$$m(t) = \int_{B(t)} \rho(t, \mathbf{x}) \, d\mathbf{x}, \qquad t \geq 0.$$

According to the *law of conservation of mass* the time derivative of $m(t)$ is zero. Thus, we obtain from (2.4) the balance equation (2.7) with $\psi = \rho$, $f = 0$, and the convective flux $\mathbf{q} = \rho\mathbf{u}$. We obtain the differential balance equation of mass, known as *continuity equation*,

$$\frac{\partial}{\partial t}\rho(t, \mathbf{x}) + \nabla \cdot (\rho(t, \mathbf{x})\mathbf{u}(t, \mathbf{x})) = 0. \tag{2.8}$$

In the following, we concentrate on incompressible fluids. In this case the volume V of the fluid at time t is conserved, hence

$$\frac{d}{dt}V(t) = \frac{d}{dt}\int_{B(t)} 1 \, d\mathbf{x} = 0, \quad t \geq 0. \tag{2.9}$$

We apply the transport theorem 2.2.1 with $\psi = 1$ to equation (2.9). For that purpose, we choose the substantial volume $B(t)$ as a ball with center $\mathbf{x}$ at time t, i.e., $B(t) = B_r(\mathbf{x})(t) := \{\Phi(t; t_0, \mathbf{x}_0) : \mathbf{x}_0 \in B_r(\mathbf{x})\}$ where $\Phi(t; t_0, \mathbf{x}_0)$ is the solution of (2.3). Then, division by its volume $|B_r(\mathbf{x})(t)|$ and $r \to 0+$ results in $\nabla \cdot \mathbf{u} = 0$ in $\Omega(t)$, since equation (2.9) is valid for all $B(t) \subset \Omega(t)$. Inserting this result in equation (2.8), the following two equations for incompressible fluids are obtained

$$\nabla \cdot \mathbf{u} = 0 \quad \text{and} \quad \frac{\partial}{\partial t}\rho(t, \mathbf{x}) + \mathbf{u} \cdot \nabla\rho(t, \mathbf{x}) = 0. \tag{2.10}$$

If in addition the density is independent of both t and $\mathbf{x}$, i.e., $\rho(t, \mathbf{x}) = \rho_0$, the second equation of (2.10) is trivially fulfilled and the continuity equation for incompressible fluids with constant density reads as

$$\nabla \cdot \mathbf{u} = 0. \tag{2.11}$$

Definition 2.3.1 (Incompressible Flow) *A flow is called* incompressible*, if equation (2.11) holds.*

The next physical property, used for the mathematical description of flows, is the conservation of momentum. The momentum $\mathbf{M} : J \to \mathbb{R}^n$ of a fluid inside a volume element $B(t)$ at a fixed time t is given by

$$\mathbf{M}(t) := \int_{B(t)} \rho(t, \mathbf{x}) \, \mathbf{u}(t, \mathbf{x}) \, d\mathbf{x}, \quad t \geq 0.$$

According to the conservation of momentum, also known as Newton's second law, the rate of change of momentum is equal to the sum $\mathbf{F} : J \times \Omega \to \mathbb{R}^n$ of all imposed forces, i.e.,

$$\frac{d}{dt} M(t) = \mathbf{F}. \tag{2.12}$$

The acting forces are divided into external and internal forces. External forces act on the fluid from the outside, such as the gravity force. In contrast, internal forces act inside the fluid such as the pressure and internal friction [Gie94]. External forces can be written as a volume integral

$$\mathbf{F}_{\text{ext}} = \int_{B(t)} \rho(t, \mathbf{x})\ \mathbf{f}(t, \mathbf{x})\ d\mathbf{x}, \tag{2.13}$$

where $\rho\ \mathbf{f}$ denotes the force density (force per unit volume). Thus, $\mathbf{f} = -g\ \mathbf{e}_3$ holds for the gravity force acting in the negative x_3-axis, where g is the gravitational acceleration.

Internal forces can be balanced by cutting out an infinitesimal fluid element and considering forces which "are placed" onto the fluid element's surface in compliance with Newton's third law. According to the hypothesis of Cauchy holds: stress depends only on the element's position and the orientation of the element's faces [Gie94]. Therefore, internal forces can be described as a surface integral

$$\mathbf{F}_{\text{int}} = \int_{\partial B(t)} \mathbf{t}(\mathbf{n}, t, \mathbf{x})\ dA,$$

where the tension $\mathbf{t}$ depends on the direction of the outer normal $\mathbf{n}$ on the surface element $\partial B(t)$, the time t, and the place $\mathbf{x}$. Note, that the tension $\mathbf{t}$ has the same unit as the pressure. The tension $\mathbf{t}$ is precisely given as

$$\mathbf{t}(\mathbf{n}, t, \mathbf{x}) = \mathbf{T}(t, \mathbf{x})\mathbf{n}, \tag{2.14}$$

where $\mathbf{T}$ is called the *total stress tensor* which we fix in the subsequent definition. For the validity of equation (2.14) we refer to [Ari62], [Spu96].

Definition 2.3.2 (Total Stress Tensor) *The tensor $\mathbf{T} : J \times \Omega \to \mathbb{R}^{n\times n}$ implicitly defined by equation (2.14) is called the* total stress tensor *or* Cauchy stress tensor*, respectively.*

Combining equation (2.13) - (2.14), the law of conservation of momentum (2.12) reads as

$$\frac{d}{dt} \int_{B(t)} \rho(t, \mathbf{x})\ \mathbf{u}(t, \mathbf{x})\ d\mathbf{x} = \int_{B(t)} \rho(t, \mathbf{x})\ \mathbf{f}(t, \mathbf{x})\ d\mathbf{x} + \int_{\partial B(t)} \mathbf{T}(t, \mathbf{x})\mathbf{n}\ dA. \tag{2.15}$$

Application of theorem 2.2.1, the product rule, the divergence theorem of Gauss on equation (2.15), and as before the choice of $B(t) = B_r(\mathbf{x})(t)$, the division by its volume and $r \to 0+$ result in the differential balance equation of momentum

$$\frac{\partial}{\partial t}(\rho\mathbf{u}) + \operatorname{div}(\rho\mathbf{u} \otimes \mathbf{u}) = \operatorname{div} \mathbf{T} + \rho\mathbf{f} \qquad \text{in } \Omega. \tag{2.16}$$

Later on, we will see that $\mathbf{T}$ depends on $\nabla\mathbf{u}$, but can also depend on powers of $\nabla\mathbf{u}$. This dependency is determined by fluid properties (see section 2.5). Thus, the total stress tensor $\mathbf{T}$ determines the order of this equation. For the remainder of this section it is assumed that $\mathbf{T}$ can be separated into the linear pressure term p and the viscous stress tensor $\mathbf{S} : J \times \Omega \to \mathbb{R}^{n\times n}$,

$$\mathbf{T} = -p\,\mathbf{I} + \mathbf{S}, \tag{2.17}$$

(for details see section 2.4). If equation (2.17) is inserted into the momentum balance equation (2.16) and the continuity equation (2.11) is added, the system of balance equations is received which is valid for the motion of an incompressible fluid

$$\begin{aligned} \tfrac{\partial}{\partial t}(\rho\mathbf{u}) + \rho\,(\mathbf{u}\cdot\nabla)\,\mathbf{u} + \nabla p &= \operatorname{div}\mathbf{S} + \rho\mathbf{f}, \\ \operatorname{div}\mathbf{u} &= 0. \end{aligned} \tag{2.18}$$

As a concrete example, the well-known stress tensor $\mathbf{S}$ for viscous incompressible Newtonian fluids is given by the constitutive equation

$$\mathbf{S} = \mu\left[\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right], \tag{2.19}$$

where μ is the *dynamical viscosity* and $(\nabla\mathbf{u})^T$ the transposed of the velocity gradient $\nabla\mathbf{u}$.

Inserting equation (2.19) into the set of balance equations (2.18) divided by ρ, the well-known Navier-Stokes equations are obtained which are valid for the motion of a viscous incompressible Newtonian fluid

$$\begin{aligned} \tfrac{\partial}{\partial t}\mathbf{u} + (\mathbf{u}\cdot\nabla)\,\mathbf{u} - \nu\Delta\mathbf{u} + \tfrac{1}{\rho}\nabla p &= \mathbf{f} \\ \operatorname{div}\mathbf{u} &= 0, \end{aligned}$$

where $\nu := \mu/\rho$ is the *kinematical viscosity*. Neglecting the viscous forces results in the Euler equations for an ideal (inviscid) fluid. Equation (2.17) then reduces to $\mathbf{T} = -p\,\mathbf{I}$.

Regarding chapter 4 of this thesis, in which two-phase flows are investigated, we remark that additional jump conditions are received. The interfacial jump conditions result from the transformation from the integral equations into the partial differential equations which express the local balances of mass and momentum.

2.4 The Total Stress Tensor

Consider a viscous incompressible fluid between two plane parallel plates separated by a distance d (see figure 2.3). The lower plate is at rest, whereas the upper one moves in the positive x_1-direction having a constant velocity $\mathbf{v}_0 = (v_0, 0, 0)$, i.e., the flow is steady. The attaining velocity profile in the gap becomes linear and the flow is called *laminar*.

In order to move the upper plate of size A with the constant velocity $\mathbf{v}_0$, a force $\mathbf{F} = (F_1, 0, 0)^T$ with

$$F_1 = \mu\,\frac{v_0}{d}\,A$$

is required, i.e., the force F_1 is proportional to the plate size A and the initial velocity v_0, but inversely proportional to the distance d [Vog95]. Then, the proportionality constant

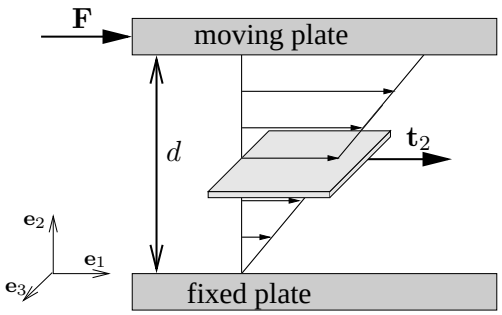


Figure 2.3: Simple Steady Shear Flow: The velocity field is given by $\mathbf{u}(\mathbf{x}) = (u_1, 0, 0)^T$ with $u_1(x_2) = v_0 x_2/d$.

is defined as the dynamical viscosity μ. The dynamical viscosity μ is a fluid property which refers to the internal friction between adjacent fluid layers.

Then, the tension $\mathbf{t}_w$ at the wall is defined as

$$\mathbf{t}_w = \frac{\mathbf{F}}{A}.$$

For a fluid layer in the steady simple shear flow, lying in the x_1x_3-plane with normal vector $\mathbf{n} = \mathbf{e}_2$, the tension vector $\mathbf{t}$ is given by

$$\mathbf{t}(\mathbf{e}_2, t, \mathbf{x}) = \left(\mu \frac{\partial u_1(x_2)}{\partial x_2}, 0, 0\right)^T. \tag{2.20}$$

According to equation (2.14), the stress vector $\mathbf{t}(\mathbf{n}, t, \mathbf{x})$ depends linearly on the direction of the external normal $\mathbf{n}$ to the surface element and the stress tensor $\mathbf{T} = (T_{ij})_{i,j=1,2,3}$. Thus, the tension $\mathbf{t}(\mathbf{e}_2, t, \mathbf{x})$ in equation (2.20) is understood as the second row of the tensor $\mathbf{T}$. For this reason, the tension vectors $\mathbf{t}(\mathbf{e}_k, t, \mathbf{x})$ for $k = 1, 2, 3$ are defined by

$$\mathbf{t}(\mathbf{e}_k, t, \mathbf{x}) := \begin{pmatrix} T_{k1} \\ T_{k2} \\ T_{k3} \end{pmatrix} = \mathbf{T}\mathbf{e}_k. \tag{2.21}$$

Then, the indices of T_{ij} are defined as follows: the first index i belongs to the normal vector of the plane which is directed to the x_i-axis; the second index is assigned to the component of the force acting in the direction of the x_j-axis (see figure 2.4).

Corresponding to the notion of the indices of the total stress tensor $\mathbf{T}$ (see definition 2.3.2) its components are designated as follows.

Definition 2.4.1 (Normal/Shear Stresses) *The components of the total stress tensor* $\mathbf{T}$ *acting in the normal direction (*$T_{ii}\ \forall\ i = 1, .., n$*) are denoted as* normal stresses*, whereas the remaining components (*$T_{ij}\ \forall\ i, j = 1, .., n$ *and* $i \neq j$*) are called* shear stresses*.*

Before we investigate more complex flows, in which the three velocity components may depend on all three coordinates and on time, we point out some general properties

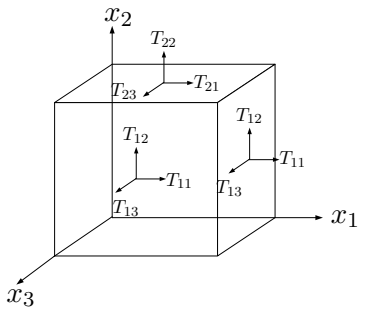


Figure 2.4: Components of the total stress tensor $\mathbf{T}$ at an infinitesimal fluid element.

for the total stress tensor. Generalized equations for the total stress tensor will be derived in section 2.5 which in case of the steady simple shear flow must simplify to the previous equation (2.20).

In addition to the momentum conservation, the *law of conservation of angular momentum* must be satisfied. Under special conditions the angular momentum can be derived from the momentum equation, but is in general independent. In an infinitesimal volume the angular momentum $d\mathbf{L}$ is given by the product of the position $\mathbf{r}$ from the origin (resp. from the axis of rotation) and the corresponding local momentum $d\mathbf{M}$, i.e., $d\mathbf{L} = \mathbf{r} \times d\mathbf{M}$. Thus, the angular momentum $\mathbf{L} : J \to \mathbb{R}^n$ in the substantial vomue $B(t)$ is given by

$$\mathbf{L}(t) = \int_{B(t)} \mathbf{r} \times (\rho\, \mathbf{u})\; d\mathbf{r}. \tag{2.22}$$

By means of the law of conservation, the rate of change of angular momentum is equal to the imposed torque $\mathbf{r} \times \mathbf{F}$, i.e., we obtain

$$\frac{d}{dt}\mathbf{L} = \int_{B(t)} \mathbf{r} \times d\mathbf{F}.$$

In the following we consider only non-polar fluids where the local force $d\mathbf{F}$ only consists of volume and surface forces. The stress tensor for polar fluids, e.g., magnetic fluids, is discussed in [Ari62].

Thus, we can use equations (2.15) and (2.22) and get for the conservation of angular momentum

$$\frac{d}{dt}\int_{B(t)} \rho\, \mathbf{r} \times \mathbf{u}\, d\mathbf{r} = \int_{B(t)} \rho\, \mathbf{r} \times \mathbf{f}\; d\mathbf{r} + \int_{\partial B(t)} \mathbf{r} \times (\mathbf{T}\mathbf{n})\; dA. \tag{2.23}$$

Applying the transport theorem 2.2.1 on the left-hand side of equation (2.23), exploiting $\frac{D}{Dt}\mathbf{r} = \mathbf{u}$ (see equation (2.2)) and using the Gauss theorem on the right-hand side ($\mathbf{r} \times (\mathbf{T}\mathbf{n}) = (\mathbf{r} \times \mathbf{T})\mathbf{n}$, where $\mathbf{r} \times \mathbf{T}$ is a tensor with the rows $\mathbf{r} \times \mathbf{t}(\mathbf{e}_k, t, \mathbf{r})$), we get

$$\int_{B(t)} \rho \left(\mathbf{r} \times \frac{D}{Dt}\mathbf{u}\right)\; d\mathbf{r} = \int_{B(t)} \Big(\mathbf{r} \times \rho\mathbf{f}\; + \nabla \cdot (\mathbf{r} \times \mathbf{T})\Big)\; d\mathbf{r}.$$

Using $\nabla \cdot (\mathbf{r} \times \mathbf{T}) = \mathbf{T}_\times + \mathbf{r} \times \nabla \cdot \mathbf{T}$ with $\mathbf{T}_\times = (T_{23} - T_{32})\mathbf{e}_1 + (T_{31} - T_{13})\mathbf{e}_2 + (T_{12} - T_{21})\mathbf{e}_3$ yields

$$\int_{B(t)} \mathbf{r} \times \left(\rho \frac{D}{Dt}\mathbf{u} - \rho \mathbf{f} - \nabla \cdot \mathbf{T} \right) \, d\mathbf{r} = \int_{B(t)} \mathbf{T}_\times \, d\mathbf{r} \tag{2.24}$$

Resulting from the conservation of momentum (2.18), the left-hand side of equation (2.24) is equal to zero. Thus, we obtain

$$\int_{B(t)} \mathbf{T}_\times \, d\mathbf{r} = 0 \qquad \Leftrightarrow \qquad \mathbf{T}_\times = 0 \qquad \Leftrightarrow \qquad \mathbf{T} = \mathbf{T}^T.$$

In summary, the tension $\mathbf{t}(\mathbf{n}, t, \mathbf{x})$ depends linearly on the normal $\mathbf{n}$, i.e., $\mathbf{t}(\mathbf{n}, t, \mathbf{x}) = \mathbf{T}(t, \mathbf{x})\mathbf{n}$ and for non-polar fluids the total stress tensor $\mathbf{T}$ is symmetric. In case of inviscid fluids, the tension vector $\mathbf{t}(\mathbf{n}, t, \mathbf{x})$ is given by $\mathbf{t}(\mathbf{n}, t, \mathbf{x}) = -p \, \mathbf{n}(t, \mathbf{x})$, where p is the thermodynamic pressure term. Therefore, it is reasonable to separate the total stress tensor $\mathbf{T}$ into the linear pressure term p and the viscous stress tensor $\mathbf{S}$, i.e.,

$$\mathbf{T} = -p \, \mathbf{I} + \mathbf{S}. \tag{2.25}$$

Besides, this separation corresponds to the case that if the fluid is at rest, only normal stresses are exerted: $\mathbf{T} = -p \, \mathbf{I}$.

2.5 Constitutive Equations

In the previous sections the balance equations of mass, momentum, and angular momentum were derived from the corresponding conservation laws. In these seven scalar equations, thirteen unknown quantities ($\mathbf{u} \in \mathbb{R}^3$, $p \in \mathbb{R}$ and $\mathbf{S} \in \mathbb{R}^{3\times3}$) are found. If the symmetry of the stress tensor is taken into consideration, the number of unknown quantities is reduced to ten in four scalar equations. To achieve a unique solution up to a constant in the pressure, further relations between the velocity field $\mathbf{u}$ and the stress tensor $\mathbf{S}$ are necessary. These relations, depending on the considered substance, are called *constitutive equations* [Gie94].

In general, there are two principal possibilities to get constitutive equations: either based on the microstructure of the substances or based on the phenomenological rheology, where basic requirements of physical principles are used to get constitutive equations describing some of the arising effects. In this section, we will follow the second strategy. In general, rheology means the study of flow and deformation, and includes everything dealing with flow behavior. However, it is common practice to restrict the meaning of the word "rheology" to the study of fundamental relations, the constitutive equations [Mac94].

First, some general concepts for constitutive equations are explained, valid for Newtonian and non-Newtonian fluids, and characteristic features of non-Newtonian fluids are presented. Afterwards, the particularities of non-Newtonian fluids will be investigated. Because of their variety (elasticity, normal stresses, memory, and recoil effects), we cannot expect that a single expression for $\mathbf{S}$ can be found, describing all these types of

fluids. The determination of all appearing material constants would be welcome, but it is impossible in most cases. Therefore, different models were developed in the literature to describe various effects. Finally, the complexity of non-Newtonian fluids is shown by means of some selected models.

2.5.1 Rate of Deformation Tensor

As outlined in section 2.4, the stress tensor $\mathbf{S}$ describes the internal friction of a fluid. Internal friction can only appear if neighboring fluid particles move with different velocities (see figure 2.3). Therefore, internal friction is related to the relative velocity and consequently, the stress tensor depends on the velocity gradient. Since each tensor of second order can be separated in its symmetric and antisymmetric part, the velocity gradient can be written as

$$\nabla \mathbf{u} = \underbrace{\frac{1}{2}\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T\right)}_{=:\mathbf{D}} + \underbrace{\frac{1}{2}\left(\nabla \mathbf{u} - (\nabla \mathbf{u})^T\right)}_{=:\mathbf{W}}. \tag{2.26}$$

Here, $\mathbf{D}$ denotes the symmetric part and $\mathbf{W}$ the antisymmetric part which has the form

$$\mathbf{W} = \begin{pmatrix} 0 & \omega_3 & -\omega_2 \\ -\omega_3 & 0 & \omega_1 \\ \omega_2 & -\omega_1 & 0 \end{pmatrix} \text{ with } \boldsymbol{\omega} = \frac{1}{2}\operatorname{rot} \mathbf{u}.$$

The meaning of $\mathbf{W}$ can be understood due to the relation

$$\mathbf{W} \cdot \mathbf{r} = \boldsymbol{\omega} \times \mathbf{r}, \quad \forall\, \mathbf{r} \in \mathbb{R}^3. \tag{2.27}$$

Due to (2.27), the antisymmetric part $\mathbf{W}$ can be described by a rigid body rotation around the $\boldsymbol{\omega}$-axis. Hence, $\mathbf{W}$ does not contribute to the internal friction. Thus, only the remaining symmetric part $\mathbf{D}$ describes the internal friction and is examined in the following.

Definition 2.5.1 (Irrotational Flow) *A flow is called* irrotational *if its velocity field is vortex free, i.e., if* $\boldsymbol{\omega} = \operatorname{rot} \mathbf{u} = 0$.

Consider two adjacent fluid particles at position $\mathbf{x}$ and $\mathbf{x}+\mathbf{h}$ with a small distance $|\mathbf{h}|$. According to the Taylor series of $\mathbf{u}$, it follows that

$$\mathbf{u}(\mathbf{x}+\mathbf{h}) = \mathbf{u}(\mathbf{x}) + \nabla \mathbf{u}(\mathbf{x}) \cdot \mathbf{h} + O(|\mathbf{h}|^2).$$

By combination of equations (2.26) and (2.27), we obtain $\nabla \mathbf{u} \cdot \mathbf{h} = \mathbf{D} \cdot \mathbf{h} + \boldsymbol{\omega} \times \mathbf{h}$, and therefore, the relative velocity $\mathbf{v}$ of the fluid particles at position $\mathbf{x}$ and $\mathbf{x}+\mathbf{h}$ is given by

$$\mathbf{v}(\mathbf{h}) := \mathbf{u}(\mathbf{x}+\mathbf{h}) - \mathbf{u}(\mathbf{x}) = \mathbf{D} \cdot \mathbf{h} + \boldsymbol{\omega} \times \mathbf{h}.$$

Due to $d\mathbf{h}/dt = \mathbf{v}(\mathbf{h})$, the tensor $\mathbf{D}$ can be interpreted by means of the relation

$$\frac{d}{dt}\mathbf{h} = \mathbf{D} \cdot \mathbf{h} + \boldsymbol{\omega} \times \mathbf{h}.$$

In order to illustrate the meaning of the tensor $\mathbf{D}$ [Böh81], we consider the time derivative of the scalar product of two substantial line elements $\mathbf{x}$ and $\mathbf{y}$

$$\begin{aligned}\frac{d}{dt}(\mathbf{x}\cdot\mathbf{y}) &= \left(\frac{d}{dt}\mathbf{x}\right)\cdot\mathbf{y}+\mathbf{x}\cdot\left(\frac{d}{dt}\mathbf{y}\right)\\ &= \mathbf{D}\mathbf{x}\cdot\mathbf{y}+(\boldsymbol{\omega}\times\mathbf{x})\cdot\mathbf{y}+\mathbf{x}\cdot\mathbf{D}\mathbf{y}+\mathbf{x}\cdot(\boldsymbol{\omega}\times\mathbf{y})\\ &= 2\,\mathbf{x}\cdot\mathbf{D}\mathbf{y} \qquad \text{(due to symmetry of } \mathbf{D}).\end{aligned}$$

Denoting the angle between the vectors $\mathbf{x}$ and $\mathbf{y}$ with $(\pi/2-\gamma)$, the scalar product can be written as $|\mathbf{x}|\,|\mathbf{y}|\cos(\pi/2-\gamma)$ and we obtain

$$\begin{aligned}\frac{d}{dt}\left(|\mathbf{x}|\,|\mathbf{y}|\cos(\pi/2-\gamma)\right) &= 2\,\mathbf{x}\cdot\mathbf{D}\mathbf{y}\\ \Leftrightarrow \left[\left(\frac{d}{dt}|\mathbf{x}|\right)|\mathbf{y}|+|\mathbf{x}|\left(\frac{d}{dt}|\mathbf{y}|\right)\right]\sin(\gamma)+|\mathbf{x}|\,|\mathbf{y}|\,\cos\gamma\,\frac{d}{dt}\gamma &= 2\,\mathbf{x}\cdot\mathbf{D}\mathbf{y}. \quad (2.28)\end{aligned}$$

For example, inserting $\mathbf{x}=\mathbf{y}=(x_1,0,0)^T$ in equation (2.28) and due to $|\mathbf{x}|=x_1$ and $\gamma=\pi/2$, we receive for the diagonal entry D_{11}

$$\frac{d}{dt}x_1 = D_{11}x_1. \quad (2.29)$$

Thus, D_{11} describes the deformation of a fluid element in direction of x_1.

Due to the symmetry of $\mathbf{D}$, the tensor $\mathbf{D}$ can also be realized as a pure deformation. Using an orthogonal transformation, we rewrite $\mathbf{D}$ in its diagonal form $\mathbf{D}=\mathrm{diag}(d_1,d_2,d_3)$. In this reference frame, the trajectories $x_i(t)$ are given according to equation (2.29) by

$$\begin{aligned}\frac{d}{dt}x_i &= d_i x_i\\ \Rightarrow \qquad x_i(t) &= e^{d_i t}x_i(0) \quad \forall\, i=1,2,3 \text{ and the initial point } x_i(0). \quad (2.30)\end{aligned}$$

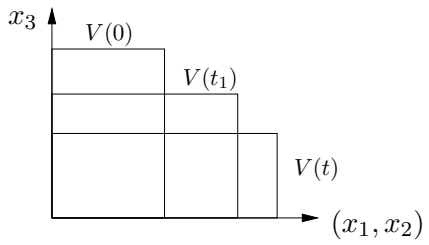
This is illustrated in the example depicted in figure 2.5(a). A fluid occupies a rectangular domain having the volume V. Considering the deformation of this volume element in time, we get in combination with equation (2.30)

$$\begin{aligned}\frac{d}{dt}V &= \frac{d}{dt}(x_1x_2x_3) = (d_1+d_2+d_3)\,V\\ &= \mathrm{tr}(\mathbf{D})\,V. \quad (2.31)\end{aligned}$$

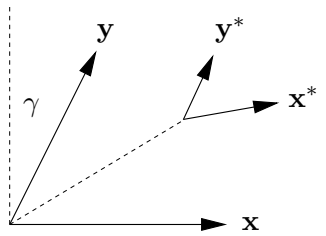
For the off-diagonal entries of $\mathbf{D}$, we consider the case $\mathbf{x}=(x_1,0,0)^T$ and $\mathbf{y}=(0,y_2,0)^T$ and insert $\mathbf{x},\mathbf{y}$ in equation (2.28). Thus, $|\mathbf{x}|=x_1$, $|\mathbf{y}|=y_2$ and $\gamma=0$, such that

$$\frac{d}{dt}\gamma = 2\,D_{12}. \quad (2.32)$$

We conclude that the principal values of $\mathbf{D}$ describe a deformation of a fluid element, whereas the off-diagonal entries of $\mathbf{D}$ describe the change of the angle between the substantial points $\mathbf{x}$ and $\mathbf{y}$ which are oriented corresponding to the coordinate directions.



(a) Main Diagonal Entries of $\mathbf{D}$. Pure elongation for a volume element V at different points in time with $0 < t_1 < t$.



(b) Off-diagonal Entries of $\mathbf{D}$. Change of the angle between two substantial line elements $\mathbf{x}$ and $\mathbf{y}$.

Figure 2.5: Meaning of the components of $\mathbf{D}$.

The off-diagonal entries of $\mathbf{D}$ are equal to half the velocity, changing the right angle (see figure 2.5).

The restriction on the diagonal form of $\mathbf{D}$ physically means that in this reference frame only elongation and compression occur, yielding the following straightforward definition.

Definition 2.5.2 (Rate of Deformation Tensor) *The tensor* $\mathbf{D} : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ *given by*

$$\mathbf{D}(\mathbf{u}) = \frac{1}{2}\left[\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right]$$

is called rate of deformation tensor.

According to equation (2.31) and due to $\operatorname{tr}(\mathbf{D}) = \operatorname{div}\mathbf{u}$, the volume change is proportional to $\operatorname{div}\mathbf{u}$. As mentioned at the beginning of this section, we search for a relation between the velocity field $\mathbf{u}$ and the stress field $\mathbf{S}$. As a result of the considerations made above, we assume that $\mathbf{S}$ is a function of the deformation tensor $\mathbf{D}$ and $\operatorname{div}\mathbf{u}$. The simplest relation for $\mathbf{S}$ is given by the linear relation

$$\mathbf{S} = 2\mu\,\mathbf{D} + \lambda\,(\operatorname{div}\mathbf{u})\;\mathbf{I},$$

with proportionality constants μ, known as the dynamical viscosity, and λ known as the Láme constant. Thus, for incompressible Newtonian fluids we obtain equation (2.19).

With the aid of these considerations, we distinguish Newtonian and non-Newtonian fluids as described by the following definition.

Definition 2.5.3 (Newtonian/ Non-Newtonian Fluids) *If the relation of the stress tensor* $\mathbf{S}$ *and the deformation tensor* $\mathbf{D}$ *is linear and the dynamical viscosity* μ *is constant (neglecting temperature and pressure effects), the fluid belongs to the class of* Newtonian fluids. *Otherwise, the fluid is called* non-Newtonian fluid.

Strictly speaking, no real fluid belongs to the class of Newtonian fluids. Nevertheless, one can in general say that fluids of low molecular weight (< 5000 [BSL02]) are approxi-

mated very well by the class of Newtonian fluids and that macromolecular fluids belong to the class of non-Newtonian fluids.

2.5.2 Rate of Shear

One approach to get constitutive equations for incompressible non-Newtonian fluids is to generalize well-known simple experiments. Following this idea, we consider the deformation tensor in the context of the steady simple shear flow. From this point of view, we introduce some additional flow quantities and generalize them to more complex flows. Before that, we introduce some tensor quantities.

The tensor invariants, which values are independent of the choice of coordinate system, of a tensor $\mathbf{D}$ of second order are given by

$$\begin{array}{rcl} I_D &=& \text{tr } \mathbf{D}, \\ II_D &=& \frac{1}{2}\left[(\text{tr } \mathbf{D})^2 - \text{tr } \mathbf{D}^2\right], \\ III_D &=& \det \mathbf{D}. \end{array} \tag{2.33}$$

Since each other tensor invariant of $\mathbf{D}$ can be constructed with the aid of these three invariants, it is sufficient to assume that the stress tensor $\mathbf{S}$ depends solely on these invariants. Due to $\text{tr } \mathbf{D} = \text{div } \mathbf{u}$ and that we only consider incompressible fluids here, the first invariant becomes $I_D = 0$ and the second one simplifies to $II_D = -1/2 \text{ tr } \mathbf{D}^2$.

In case of the steady simple shear flow example, we obtain the deformation tensor

$$\mathbf{D} = \frac{1}{2}\begin{pmatrix} 0 & \frac{\partial u_1}{\partial x_2} & 0 \\ \frac{\partial u_1}{\partial x_2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \text{ with its invariants } \begin{cases} I_D &=& 0, \\ II_D &=& -\frac{1}{4}\left(\frac{\partial u_1}{\partial x_2}\right)^2, \\ III_D &=& 0. \end{cases} \tag{2.34}$$

The component $D_{21} = 1/2 \ \partial u_1/\partial x_2$ describes the change in velocity perpendicular to the flow direction (see figure 2.3). If we take a fluid plane out of the steady simple shear flow (dotted line in figure 2.6(a)), the component D_{21} can be interpreted via equation (2.32) as rate of change of the angle. Thereby, the flow is produced by deformation (see figure 2.6(a)) and rotation caused by shear [3] (see figure 2.6(b)).

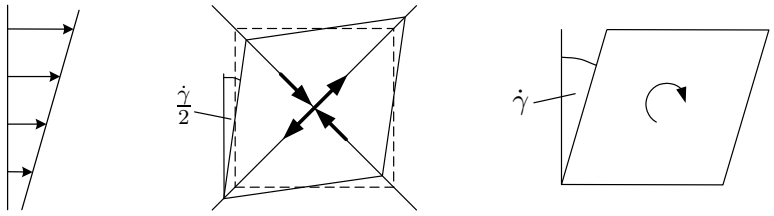
Then, the quantity $\dot{\gamma} := 2\,|D_{21}|$ is defined as *rate of shear* and describes the change in velocity perpendicular to the flow direction. By means of the invariants we express this quantity more generally as $\dot{\gamma} = \sqrt{-4\ II_D}$ or $\dot{\gamma} = \sqrt{2\ \text{tr}(\mathbf{D}^2)}$, respectively. Based on these considerations we define the shear rate for more complex flows.

Definition 2.5.4 (Rate of Shear) *The quantity* $\dot{\gamma} := \sqrt{2\ tr(\mathbf{D}^2)}$ *is called* rate of shear.

In accordance with section 2.4, equation (2.20) combined with equation (2.21) and definition 2.5.2 (resp. definition 2.5.4), a relation for incompressible Newtonian fluids is obtained as

$$S_{21}(t, \mathbf{x}) = \mu\ \dot{\gamma}(t, \mathbf{x}) = 2\,\mu\ D_{21}(t, \mathbf{x}), \tag{2.35}$$

[3] This is different to the rigid rotation which is described by the antisymmetric tensor $\mathbf{W}$.



(a) Deformation

(b) Rotation caused by shear

Figure 2.6: The steady simple shear flow is produced by a superposition of deformation and rotation caused by shear [Böh81].

where the viscosity μ is constant. Note, that for the steady simple shear flow the static pressure is constant, thus $\mathbf{T} = \mathbf{S}$ by suitable normalization. Equation (2.35) expresses that the stress in a given fluid element at a certain time t depends only on the current deformation/translation of this element and not on the movement at other time states. Additionally, the stress only depends on the deformation of this fluid element and not on the deformation of adjacent elements which means that there is only *local stress*. Actually, higher derivatives of the velocity gradient are irrelevant. This causes the local stress being proportional to the shear rate $\dot{\gamma}$.

In case of non-Newtonian fluids the situation is more complex [Gie94], [TR00]. In general, it is possible that the movement of a fluid element not only depends on the current time, but also on the movements in the past, i.e., the deformation history of the fluid element has to be taken into account. In this case the fluid is characterized by so-called memory effects.

2.5.3 General Principles for Constitutive Equations

Before we exemplify some constitutive equations in the subsections to follow, we fix some general principles which constitutive equations have to satisfy [TR00]:

- *Principle of determinism.* The stress is determined by its flow history, i.e., the motion up to and including the present time determines a unique symmetric stress tensor.
- *Principle of local action.* The fluid only shows local stress effects, i.e., the deformation of a fluid element does not depend on the deformation of adjacent fluid elements.
- *Principle of material frame indifference.* The stress is independent of the reference frame, i.e., no stress is created by translation ar rotation of a material element.

Furthermore, in order to obtain constitutive equations, internal constraints, e.g., incompressibility or certain assumption on the fluid are taken into account.

2.5.4 Incompressible Pure Viscous Fluids

In this subsection, we consider the constitutive equation for an incompressible pure viscous fluids, where the constitutive equation has to satisfy the principles of subsection 2.5.3. For those fluids constitutive equations can be defined by the assumption they depend only on the deformation tensor $\mathbf{D}$ [Gie94] which combined with equation (2.25) results in

$$\mathbf{T} = -p\,\mathbf{I} + \mathbf{f}(\mathbf{D}) \tag{2.36}$$

with $\mathbf{f}(\mathbf{0}) = \mathbf{0}$, and $\mathbf{f}$ is an isotropic tensor function. Thus, $\mathbf{S} = \mathbf{f}(\mathbf{D})$ with $\mathbf{f}(\mathbf{0}) = \mathbf{0}$. The linear relation $\mathbf{S} = 2\ \mu\ \mathbf{D}$ is the constitutive equation for incompressible pure viscous Newtonian fluids, as we saw in subsection 2.5.1. However, a nonlinear relation is also conceivable which we consider later in this subsection.

Linear Relation: Generalized Newtonian Fluids

The linear model $\mathbf{S} = 2\ \mu\ \mathbf{D}$ is extended by replacing the constant viscosity by a function depending on the shear rate. Such fluids are often called *generalized Newtonian fluids*. In coherence with equation (2.35), the viscosity of a fluid in a steady simple shear flow is defined as

$$\mu(\dot{\gamma}) := \frac{S_{21}}{\dot{\gamma}}.$$

Thus, the viscosity $\mu(\dot{\gamma})$ can be interpreted as *shear dependent viscosity*.

With the aid of this viscosity definition, we can classify the generalized Newtonian fluids in several subclasses and explain their different flow behaviors (see figure 2.7). In case of the generalized Newtonian fluids, we mainly distinguish two different flow behaviors. The first one appears if the fluid becomes more viscous with increasing shear rate. This property is often called *shear thickening*. The opposite property, i.e., the viscosity decreases with increasing shear rate, is called *shear thinning*. These fluids are also called *dilatant* and *pseudoplastic*, respectively. For the sake of completeness, we mention a third class, where the fluid does not flow until a critical stress is exerted. These fluids are called *viscoplastic fluids*.

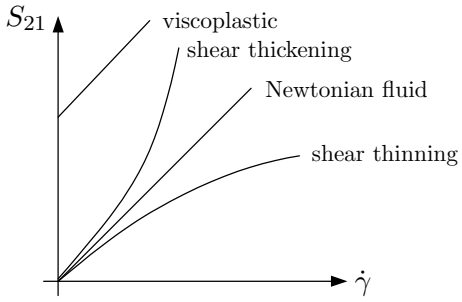


Figure 2.7: Stress S_{21} versus shear rate.

The viscosity of Newtonian fluids is a material constant (see definition 2.5.3), whereas the viscosity of non-Newtonian fluids is characterized by a nonlinear relation of the stress and the shear rate. The most simple model describing this viscosity effect is known as the "Power Law" model of Ostwald and de Waele and is given by

$$\mu(\dot{\gamma}) = K\dot{\gamma}^{m-1},$$

with empirical constants K, m. The dimensionless constant m indicates the type of fluid. If $m > 1$, the fluid belongs to the class of shear thickening fluids, if $0 < m < 1$, the fluid belongs to the class of shear thinning fluids, and in case of $m = 1$ the model reduces to the Newtonian model. Evidently, the constant K has the unit of viscosity and in case of $m = 1$, K corresponds to the viscosity μ.

The Power Law model involves some difficulties: in case of shear thinning fluids, the viscosity converges to zero with increasing shear rate and in case of shear thickening fluids, the viscosity converges to infinity with decreasing shear rate, respectively. However, in reality the viscosity approaches a constant value μ_0 for small shear rates, the so-called *zero-shear-rate viscosity*, and in case of very high shear rates the viscosity becomes independent and approaches μ_∞, the so-called *infinite-shear-rate viscosity*. Therefore, more complex models were developed which reflect these observations [BAH77].

An especially useful form was introduced by Carreau [BAH77, Tan88], setting

$$\mu(\dot{\gamma}) = \mu_\infty + (\mu_0 - \mu_\infty)\left[1 + (\lambda\dot{\gamma})^2\right]^{(m-1)/2}. \tag{2.37}$$

Here, the zero-shear-rate viscosity μ_0, the infinite-shear-rate viscosity μ_∞, λ, and m are constants which are determined by experimental investigations and characterize the used fluid. As before, the dimensionless constant m indicates the type of fluid. Additionally, several other models exist [BAH77, Gie94].

Nonlinear Relation: Reiner-Rivlin Equation

Here, we assume that the function $\mathbf{f}(\mathbf{D})$ in equation (2.36) is quadratic in $\mathbf{D}$, i.e.,

$$\mathbf{S} = \alpha_1(II_D, III_D)\mathbf{D} + \alpha_2(II_D, III_D)\mathbf{D}^2,$$

with scalar functions α_1 and α_2, which only depend on the non-vanishing invariants II_D and III_D of $\mathbf{D}$ (see equation (2.33)). This general equation is called *Reiner-Rivlin equation*. In comparison to the previously discussed linear case, it is evident that the function α_1 corresponds to the viscosity function μ. Therefore, the Reiner-Rivlin equation is often written as

$$\mathbf{S} = 2\,\mu(\dot{\gamma})\,\mathbf{D} + 4\,\xi(\dot{\gamma})\,\mathbf{D}^2, \tag{2.38}$$

with the so-called *cross viscosity* $\xi(\dot{\gamma})$ [Gie94].

Once more, consider the simple shear flow. In this case, the deformation tensor $\mathbf{D}$ and its invariants are given as in (2.34), combined with the definition of the shear rate we get

$$\mathbf{D} = \frac{\dot{\gamma}}{2}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad \mathbf{D}^2 = \frac{\dot{\gamma}^2}{4}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Inserting in equation (2.38) yields

$$\mathbf{S} = \begin{pmatrix} \xi(\dot{\gamma})\dot{\gamma}^2 & \mu(\dot{\gamma})\dot{\gamma} & 0 \\ \mu(\dot{\gamma})\dot{\gamma} & \xi(\dot{\gamma})\dot{\gamma}^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{2.39}$$

From the experimental point of view, it is only possible to measure stress differences, i.e., it is reasonable to introduce the *normal stress differences*

$$N_1 := S_{11} - S_{22}, \quad N_2 := S_{22} - S_{33}, \quad N_3 := S_{11} - S_{33} = N_1 + N_2.$$

In particular, the first normal stress difference is proportional to $\dot{\gamma}^2$ [BAH77], and therefore, it is common to define the *normal stress coefficients* by

$$\psi_1(\dot{\gamma}) := N_1/\dot{\gamma}^2, \quad \psi_2(\dot{\gamma}) := N_2/\dot{\gamma}^2. \tag{2.40}$$

Determining the normal stress coefficients of the stress tensor (2.39) results in $\psi_1 = 0$ and $\psi_2 = \xi(\dot{\gamma})$. Thus, equation (2.38) can be written in the form

$$\mathbf{S} = 2\,\mu(\dot{\gamma})\,\mathbf{D} + 4\,\psi_2(\dot{\gamma})\,\mathbf{D}^2. \tag{2.41}$$

The assumption that the constitutive equation depends only on the stress tensor $\mathbf{D}$, and not on $\nabla\mathbf{u}$, results in the fact that the Reiner-Rivlin equation is only able to describe fluids in steady, homogeneous and irrotational flows. Furthermore, with the prospect of the next subsections we point out that the Reiner-Rivlin equation defined for pure viscous fluids becomes a borderline case of viscoelastic fluids [Gie94].

2.5.5 Other Models

In case of incompressible pure viscous fluids, we presented constitutive equations on the foundation of differential models, where the stress is expressed as power series involving increasing powers of the deformation tensor. Continuing this conception leads to the usage of *convected derivatives* based on the application of the invariance of material properties with respect to the frame reference. These time derivatives have to satisfy the principles of subsection 2.5.3. This method will be presented using the two models *retarded motion expansion* and *Criminale-Ericksen-Filbey (CEF) equation.*

Integral-type models are another approach to get constitutive equations. Rheologists use integral formulations whereby the stress at any location and time depends on the entire past history of the local deformation. For a historical perspective on the evolution of rheology, see [Dor02].

As stated in subsection 2.5.3, an important requirement of constitutive equations is that they have to be frame indifferent. In order to obtain objective equations, it is important to fix the reference frame. For this purpose, several opportunities exist, which is the primary reason for the variety of constitutive equations. In particular, three different frames are used:

(i) *Laboratory frame:* this frame is a fixed frame

(ii) *Corotational frame:* this frame is moving and rotating with the fluid

(iii) *Codeformational frame:* this frame has the same purpose as the corotational, but additionally can change in unit size if the fluid element is deformed.

The equations received by the usage of the codeformational frame are called *memory integral expansions* [BAH77] and are applicable to most of the relevant physical problems with non-Newtonian fluids. They are defined by special integral kernels depending on selected parameters. Even more general models can be obtained by expanding the number of selected parameters. These memory integral expansions pass into simpler models if they are restricted by physical constraints (see figure 2.8).

The corotational description leads to nonlinear models like the well-known *Oldroyd 8-constant model*, the retarded motion expansion, and the CEF model. Before describing these models in detail, we shortly discuss *viscoelastic fluids* and the first (linear) approaches dealing with these type of fluids.

Linear Viscoelastic Models

In addition to viscous effects, non-Newtonian fluids are able to show elastic effects. If both effects are predominant, they are combined in the notion *viscoelastic effects*. Pure elastic effects can be described with the aid of Hooke's law: the principle that, within the elastic limit, stress applied to a solid is proportional to the produced strain.

First approaches to achieve constitutive equations for linear viscoelastic fluids date back to Maxwell [BAH77]. The Maxwell model combines the Newtonian law for viscous fluids and the Hookean law for elastic fluids. This model is often interpreted by mechanical analogies, since it has the same form as a model consisting of a spring and a dashpot connected in series, where a dashpot consists of a piston that moves in a cylinder containing a Newtonian fluid. By analogy with mechanical considerations a number of sophisticated networks of springs and dashpots were developed and result in different constitutive equations, e.g., Jeffreys model. Later on, all these models were included in the *general linear viscoelastic model* which can be written in the following form

$$\mathbf{S} = -\int_{\infty}^{t} G(t-t')\mathbf{D}(t')\,dt',$$

where $G(t-t')$ is the relaxation modulus. For more details, see for example [BAH77]. This equation can be used, e.g., for the description of shear flows or elongational flows, but it does not allow to describe oscillating normal stresses in shear flows, since the normal stresses are second-order effects (see the remarks to the Reiner-Rivlin equation (2.41)).

Retarded Motion Expansion

The retarded motion expansions were developed on the foundation of a corotational reference frame. A universal description was made available by the *corotational memory*

integral expansions, which presents the stress tensor as an infinite series of integrals of increasing complexity. Assuming that the velocity gradient is changing slowly in time and that the flow is independent on the past history, the retarded motion expansion is given by the differential model [BAH77]

$$\mathbf{S} = \underline{b_1\mathbf{D} - b_2\mathbf{D}' - [b_{11}(\mathbf{D}\cdot\mathbf{D})]} - b_3\mathbf{D}'' - b_{12}\left[\mathbf{D}\cdot\mathbf{D}' + \mathbf{D}'\cdot\mathbf{D}\right] - b_{1:11}(\mathbf{D}:\mathbf{D})\mathbf{D} + \ldots \quad (2.42)$$

with the *corotational* or *Jaumann derivatives*

$$\begin{aligned}\mathbf{D}' &= \frac{D}{Dt}\mathbf{D} - \mathbf{W}\cdot\mathbf{D} + \mathbf{D}\cdot\mathbf{W},\\ \mathbf{D}'' &= \frac{D}{Dt}\mathbf{D}' - \mathbf{W}\cdot\mathbf{D}' + \mathbf{D}'\cdot\mathbf{W},\end{aligned}$$

and the substantial derivative

$$\frac{D}{Dt}\mathbf{D} = \frac{\partial}{\partial t}\mathbf{D} + \mathbf{u}\cdot\nabla\mathbf{D}.$$

If a fluid flow can be described by the first linear term and the next two quadratic terms (underlined terms in equation (2.42)) alone, the fluid is called *second order fluid.* The scalars $b_1, b_2, b_{11}, \ldots$ are material parameters where the coefficient b_1 in case of an incompressible Newtonian fluid corresponds to the zero-shear viscosity μ_0.

With this model qualitative assessments of secondary flows are possible. Furthermore, it is possible to use more complex flows for measuring the zero-shear viscosity and the normal stress coefficients. This is of interest, since the measurement of the zero-shear viscosity is extremely difficult [BAH77].

Criminale-Ericksen-Filbey Equation

Criminale, Ericksen, and Filbey observed that for special flow types the deformation tensor $\mathbf{D}$ and the derivative $\mathbf{D}'$ could always be put in a certain form. Because of the kinematic simplicity of steady shear flows, the products in equation (2.42) can be expressed only in terms of $\mathbf{I}, \mathbf{D}$, and $\mathbf{D}'$ [BAH77]. Finally, equation (2.42) simplifies to the Criminale-Ericksen-Filbey Equation:

$$\mathbf{S} = 2\,\mu(\dot\gamma)\mathbf{D} + [\psi_1(\dot\gamma) + 4\psi_2(\dot\gamma)]\,\mathbf{D}^2 - \psi_1(\dot\gamma)\mathbf{D}', \quad (2.43)$$

in which ψ_1 and ψ_2 are material functions depending on the shear rate $\dot\gamma$ and indeed have the meanings of the normal stress differences defined in equation (2.40). Thus, the Reiner-Rivlin equation is contained in the CEF-equation, since for steady-state flows that are homogeneous and irrotational ($\mathbf{W} = 0$), all corotational derivatives $\mathbf{D}', \mathbf{D}'', \ldots$ are zero and we receive equation (2.41).

In addition to the Jaumann derivatives it is also admitted to define the *convected* or *Oldroyd derivative* [Gie94] which is defined as follows

$$\mathbf{D}' = \frac{D}{Dt}\mathbf{D} - \left[(\nabla\mathbf{u})^T\cdot\mathbf{D} + \mathbf{D}\cdot(\nabla\mathbf{u})\right]$$

This derivative is often cited in connection with the *Rivlin-Ericksen tensors* which are defined by the recursion

$$\mathbf{A}^{n+1} = \frac{D}{Dt}\mathbf{A}^n - \left[(\nabla \mathbf{u})^T \cdot \mathbf{A}^n + \mathbf{A}^n \cdot (\nabla \mathbf{u})\right]$$

with the initial tensor $\mathbf{A} = \mathbf{I}$. Then, $\mathbf{A}^1$ is the first Rivlin-Ericksen tensor and $A^1 = 2\mathbf{D}$ [Tan88]. The CEF-equation is also often cited using the convected derivative instead of the Jaumann derivative.

2.6 Conclusion

This chapter was motivated by some experiments showing completely different behavior for Newtonian and non-Newtonian fluids. Here, we want to point out which constitutive equations can be used in order to describe them.

The Weissenberg effect (see figure 1.1) can be described by the presence of nonzero normal stresses. In polymeric fluids the first normal stress differences are much larger than the second normal stress differences. In particular, the second normal stress difference is normally observable in situations where the first normal stress difference has no effect [BAH77]. Therefore, the Weissenberg effect can be well described with the CEF-equation (2.43). The secondary flow in rotating lid system (see figure 2.1) can be qualitatively described with equation (2.42) of second order, whereas the extrudate swell (see figure 2.2) cannot be described by the here discussed models. Finally, we summarize in figure 2.8 the relations between the discussed and some directly related models [BAH77].

In the next chapter we concentrate on generalized Newtonian fluids, in particular on flow of *incompressible pure viscous fluids with vanishing normal stress differences* which can be described by the following set of equations

$$\begin{aligned} \tfrac{\partial}{\partial t}(\rho \mathbf{u}) + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} &= \operatorname{div} \mathbf{S} - \nabla p + \rho \mathbf{f}, && \text{in } [0,T] \times \mathbb{R}^n \\ \operatorname{div} \mathbf{u} &= 0, && \text{in } [0,T] \times \mathbb{R}^n \\ \mathbf{u}_{|_{t=0}} &= \mathbf{u}_0, && \text{in } \mathbb{R}^n \end{aligned} \tag{2.44}$$

with the stress tensor $\mathbf{S} = 2\mu(\dot\gamma)\mathbf{D}$, the deformation tensor $\mathbf{D} = \frac{1}{2}\left[\nabla \mathbf{u} + (\nabla \mathbf{u})^T\right]$, and the shear rate $\dot\gamma = \sqrt{2 \operatorname{tr}(\mathbf{D}^2)}$.

For the viscosity function $\mu(\dot\gamma)$ several models were given (see section 2.5.4). Here, we recall the Carreau model (see equation (2.37))

$$\mu(\dot\gamma) = \mu_\infty + (\mu_0 - \mu_\infty)\left[1 + (\lambda\dot\gamma)^2\right]^{(m-1)/2}.$$

In this context, the following question arises: for which exponents m does a local (in time) strong solution exist for the system (2.44). This question will be treated in the forthcoming chapter.

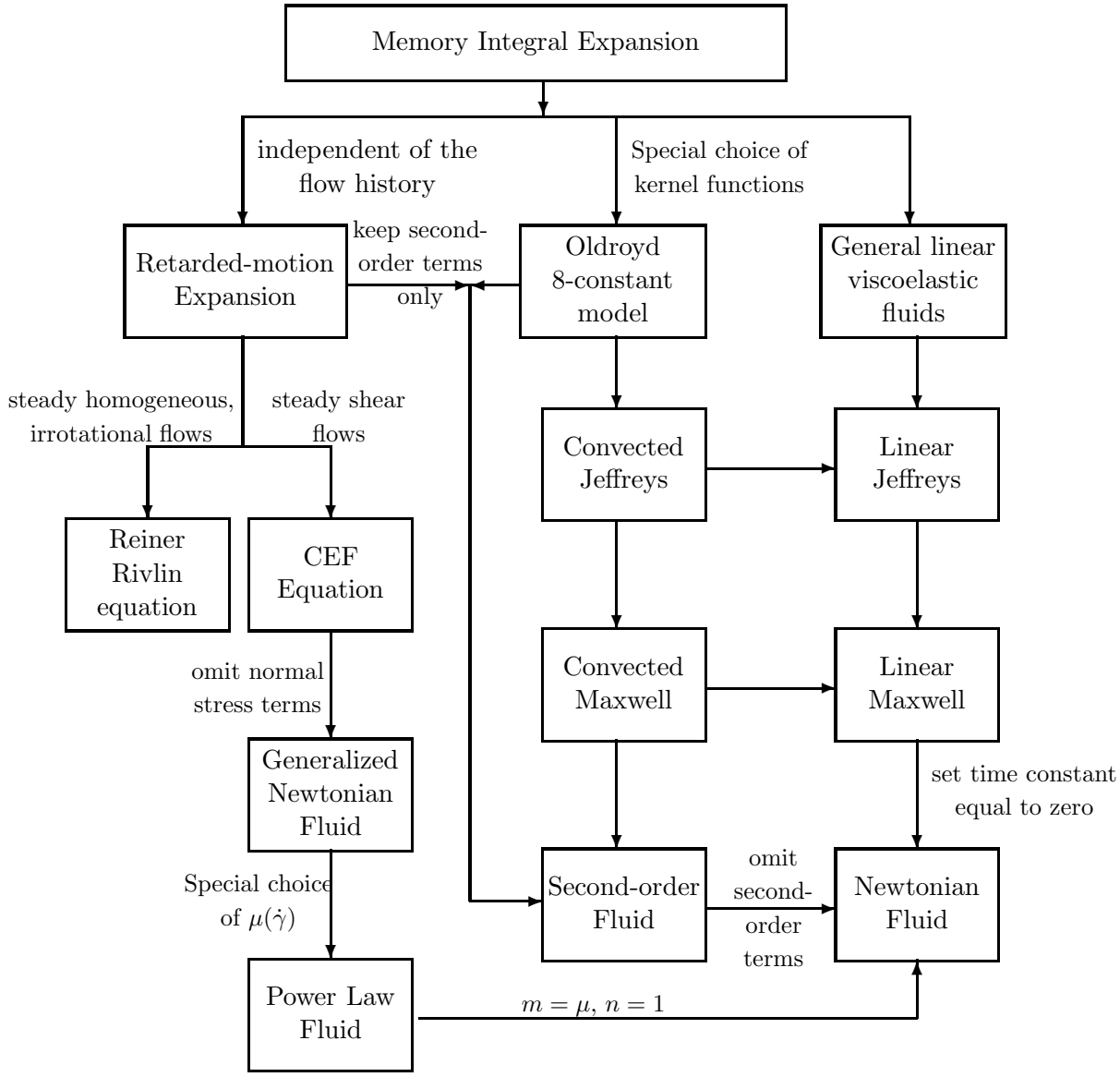


Figure 2.8: Relations among rheological equations of state [BAH77].

Chapter 3

Local Strong Solvability of Non-Newtonian Flow Problems

In this chapter, we concentrate on generalized Newtonian fluids: fluids, of which the flow behavior is mainly based on the variation of viscosity. As in section 2.5.4, the model is acquired by simply replacing the constant viscosity μ by a function $\mu(\dot{\gamma})$ depending on the shear rate $\dot{\gamma}$. We recall that $\dot{\gamma} = \sqrt{2\,\mathrm{tr}(\mathbf{D}^2)}$ (see definition 2.5.4) which is equal to $\dot{\gamma} = \sqrt{2}\,\|\mathbf{D}\|$, where

$$\|\mathbf{D}\| = \Big(\sum_{i,j=1}^{n} d_{ij}^2\Big)^{1/2} \text{ for } \mathbf{D} = (d_{ij})$$

denotes the Hilbert-Schmidt norm (also called Frobenius norm) of $\mathbf{D}$. From the model of Carreau, which is given by equation (2.37), we obtain with $\mu_\infty = 0$, $\lambda = \frac{1}{\sqrt{2}}$, and $m = k + 1$ the model

$$\mu(\|\mathbf{D}\|^2) = \mu_0 \left(1 + \|\mathbf{D}\|^2\right)^{\frac{k-2}{2}} \tag{3.1}$$

which is often quoted as standard model in the mathematical literature (see section 3.4). In order to simplify some of the computations below, it is preferable to consider μ as a function of $\|\mathbf{D}\|^2$.

Considering different models, in particular the standard model (3.1), the question arises: for which exponents, respectively for which k, does a local strong solution on $J = [0, \tau]$ for some $\tau > 0$ of the following system exist,

$$\begin{array}{rcll} \frac{\partial}{\partial t}(\rho\mathbf{u}) + \mathrm{div}\,(\rho\mathbf{u}\otimes\mathbf{u}) &=& \mathrm{div}\,\mathbf{S} - \nabla p + \rho\mathbf{f}, & \text{in } J\times\mathbb{R}^n \\ \mathrm{div}\,\mathbf{u} &=& 0, & \text{in } J\times\mathbb{R}^n \\ \mathbf{u}_{|_{t=0}} &=& \mathbf{u}_0, & \text{in } \mathbb{R}^n. \end{array} \tag{3.2}$$

As described before, $\mathbf{u}(t,\mathbf{x})$ denotes the velocity of the fluid, $p(t,\mathbf{x})$ the pressure, $\mathbf{S} = 2\,\mu(\|\mathbf{D}\|^2)\mathbf{D}$ the stress tensor, and $\mathbf{D}(\mathbf{u}) = \frac{1}{2}\left[\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right]$ the deformation tensor. The function $\mathbf{f}$ describes external forces and $\mathbf{u}_0$ the initial velocity. In the following, we assume that the density $\rho > 0$ is constant and then w.l.o.g. $\rho = 1$.

We start with some notations which will be used throughout this chapter, and recall some basic definitions. Furthermore, we collect some known results which are needed throughout the proof of our main result. In section 3.3 we formulate the main result (see theorem 3.3.1) and give the proof in the subsections to follow. Finally, an overview about related existence results in the literature is given. We mention that our result holds in the whole space $\mathbb{R}^n$, whereas the most literature is given for problems in domains.

3.1 Notations

Let J denote a time interval, $J = [0, \tau]$ for $\tau > 0$. Let further X and Y be Banach spaces endowed with their norms $|\cdot|_X$ resp. $|\cdot|_Y$. The symbol $\mathcal{B}(X, Y)$ denotes the space of all bounded linear operators from X to Y and let $\mathcal{B}(X) := \mathcal{B}(X, X)$. The spectrum of a linear operator A in X is designated by $\sigma(A)$, its resolvent set by $\rho(A)$. The domain of an operator A is denoted by $D(A)$, the range by $R(A)$, and the null space by $N(A)$. If A is a closed operator, D_A denotes the domain of A equipped with the graph norm.

Furthermore, we denote by $L_p(J; X)$, $1 \leq p < \infty$ the space of all Bochner measurable functions $\phi : J \to X$ equipped with the norm $|\phi|_{L_p(J;X)} = \left(\int_J |\phi(t)|_X^p \, dt\right)^{1/p}$. If $n \in \mathbb{N}$ is the space dimension, we define by analogy the space $L_p(\mathbb{R}^n; X)$ of all Bochner measurable functions $\phi : \mathbb{R}^n \to X$ equipped with corresponding norm. In the scalar case $X = \mathbb{R}$ we usually omit the image space $L_p(\mathbb{R}^n) = L_p(\mathbb{R}^n; \mathbb{R})$. For the definition of the Bochner integral we refer to [AF03]. The space $L_p(\mathbb{R}^n; \mathbb{R}^n)$ coincides with $L_p(\mathbb{R}^n) \times \ldots \times L_p(\mathbb{R}^n)$ endowed with the norm $|\boldsymbol{\phi}|_{L_p(\mathbb{R}^n;\mathbb{R}^n)} := \left(\sum_{i=1}^n |\phi_i|_p^p\right)^{1/p}$.

The space $\mathcal{D}(\mathbb{R}^n; X)$ denotes the space of all X-valued C^∞-functions with compact support on $\mathbb{R}^n$, whereas the *Schwartz space* $S(\mathbb{R}^n; X)$ consists of all infinitely differentiable, rapidly decreasing X-valued functions [Ama95, p. 129].

Further, let $\alpha = (\alpha_1, \ldots, \alpha_n)$ be an $n-$tuple of nonnegative integers and $|\alpha| = \sum_{j=1}^n \alpha_j$. Since we use the differential operator within the framework of the Fourier transform, it is preferable to define the operator as $D_j = -i \, \partial/\partial x_j$ with the complex number i, then $D^\alpha = D_1^{\alpha_1} \cdots D_n^{\alpha_n}$ is the differential operator of order $|\alpha|$. For $m \in \mathbb{N}$ is $C^m(\mathbb{R}^n)$ the space of all functions ϕ which, together with all their partial derivatives $D^\alpha \phi$ of order $|\alpha| \leq m$, are continuous on $\mathbb{R}^n$. Let Ω be a measurable subset of $\mathbb{R}^n$. The subspace $C_0^\infty(\Omega)$ consists of all functions in $C_0^\infty(\Omega)$ that have compact support in Ω.

The complex scalar product is denoted by $(\cdot, \cdot)$, whereas the real scalar product is designated by $\langle \cdot, \cdot \rangle$. Finally, by C and M we denote various constants which may differ from line to line.

3.2 Preliminaries

In order to fix our notation, we start this section with some well-known definitions about differential operators with constant coefficients, more generally pseudo-differential operators on $L_p(\mathbb{R}^n)$. Additionally, we introduce the vector-valued Laplace transformation.

This part is mainly based on [ABHN01], [Ama95], [DHP03]. We recall the definition of sectorial operators, $\mathcal{R}$-bounded operator families, and operators which admit a bounded $\mathcal{H}^\infty$-calculus as well as semi-Fredholm operators. Furthermore, we collect some theorems which we need in the proof of theorem 3.3.1.

We start with the basic definition of symbols.

Definition 3.2.1 (Symbol) *We call $\mathcal{A} \in C^\infty(\mathbb{R}^n)$ a* symbol *if for some $m > 0$ and some $\rho \in [0,1]$ there exists a constant C_α such that*

$$|D^\alpha \mathcal{A}(\boldsymbol{\xi})| \leq C_\alpha \left(1 + |\boldsymbol{\xi}|\right)^{m-\rho|\alpha|}, \qquad \boldsymbol{\xi} \in \mathbb{R}^n,$$

for each multi-index $\alpha \in \mathbb{N}_0^n$.
Evidently, each polynomial of order m is a symbol for $\rho = 1$.

For $f \in L_1(\mathbb{R}^n)$, the *Fourier transform* $\mathcal{F}f$ is defined as

$$\mathcal{F}f(\boldsymbol{\xi}) = \int_{\mathbb{R}^n} e^{-i\mathbf{x}\cdot\boldsymbol{\xi}} f(\mathbf{x})\, d\mathbf{x}, \qquad \boldsymbol{\xi} \in \mathbb{R}^n.$$

According to the *Fourier inversion theorem* the Fourier transform is an isomorphism on $S(\mathbb{R}^n)$, [Yos80] and the *inverse Fourier transform* $\mathcal{F}^{-1}f$ is given by

$$\mathcal{F}^{-1}f(\boldsymbol{\xi}) = (2\pi)^{-n} \int_{\mathbb{R}^n} e^{i\mathbf{x}\cdot\boldsymbol{\xi}} f(\mathbf{x})\, d\boldsymbol{\xi}, \qquad \boldsymbol{\xi} \in \mathbb{R}^n.$$

Definition 3.2.2 (Pseudo-differential Operator) *For a symbol $\mathcal{A}(\boldsymbol{\xi})$ we define the* pseudo-differential operator $\mathcal{A}(D)$ *associated to $\mathcal{A}(\boldsymbol{\xi})$ by*

$$\mathcal{A}(D)u(\mathbf{x}) := \int_{\mathbb{R}^n} e^{i\mathbf{x}\cdot\boldsymbol{\xi}} \mathcal{A}(\boldsymbol{\xi}) \mathcal{F}u(\boldsymbol{\xi})\, d\boldsymbol{\xi}, \qquad \mathbf{x} \in \mathbb{R}^n, u \in S(\mathbb{R}^n),$$

where $\mathcal{F}u$ denotes the Fourier transform of u.

Definition 3.2.3 (L_p-Realization) *Let $f \in L_p(\mathbb{R}^n)$ and $1 \leq p < \infty$. The operator A defined by*

$$\begin{aligned} Af &:= \mathcal{F}^{-1}(\mathcal{A}(\boldsymbol{\xi})\mathcal{F}f), \\ \mathcal{D}(A) &:= \left\{\mathbf{f} \in L_p(\mathbb{R}^n) : \mathcal{F}^{-1}(\mathcal{A}(\boldsymbol{\xi})\mathcal{F}f) \in L_p(\mathbb{R}^n)\right\} \end{aligned}$$

is called the realization of $\mathcal{A}(D)$ in $L_p(\mathbb{R}^n)$*, or* L_p-realization*, respectively.*

Note that, whenever $\mathcal{A}(\boldsymbol{\xi})$ is a symbol, the L_p-realization A is a closed operator [ABHN01], [DHP03].

By the elementary relation $\mathcal{F}(Du) = \boldsymbol{\xi}\mathcal{F}u$, recall $D = -i\,(\partial/\partial\xi_1, \ldots, \partial/\partial\xi_n)$, the pseudo-differential operator $\mathcal{A}(D)$ is a differential operator of order m with constant coefficients $a_\alpha \in \mathbb{C}$, i.e.,

$$\mathcal{A}(D)u = \sum_{|\alpha| \leq m} a_\alpha D^\alpha u, \qquad u \in D_A$$

when $\mathcal{A}$ is the polynomial of order m.

Next, we define the vector-valued Laplace transform and recall Poincaré's inequality.

Definition 3.2.4 (Laplace Transform) *Let X be a Banach space. Then, for $u \in L_{1,loc}(\mathbb{R}_+; X)$ of exponential growth, i.e., $\int_0^\infty e^{\omega t} |u(t)| \, dt < \infty$ with some $\omega \in \mathbb{R}$, the* Laplace transform *is defined by*

$$\tilde{u}(\lambda) = \int_0^\infty e^{-\lambda t} u(t) \, dt, \qquad Re\, \lambda \geq \omega.$$

Lemma 3.2.1 (Poincaré's Inequality) *[Eva98, p.275] Let Ω be a bounded, connected, open subset of $\mathbb{R}^n$, with a C^1 boundary $\partial\Omega$. Assume $1 \leq p \leq \infty$. Then there exists a constant C, depending on n, p, and Ω, such that*

$$\left| \pi - \frac{1}{|\Omega|} \int_\Omega \pi \, d\mathbf{x} \right|_{L_p(\Omega)} \leq C \, |\nabla \pi|_{L_p(\Omega)}$$

for each function $\pi \in W_p^1(\Omega)$.

Furthermore, we need the following result concerning the divergence operator. It is well-known that the operators div and ∇ are connected by duality principle, see for example [Soh01]. The dual is denoted by " $*$ ". A vector-valued version of the divergence operator is given by the following theorem which is proved in Escher, Prüss, and Simonett [EPS03]. Below, we denote by $\dot{H}_p^1(\mathbb{R}^n)$ the space

$$\dot{H}_p^1(\mathbb{R}^n) = \left\{ f \in H_{p,\mathrm{loc}}^1(\mathbb{R}^n) : \ \nabla f \in L_p(\mathbb{R}^n) \right\}. \tag{3.3}$$

Moreover, $\dot{H}_p^{-1}(\mathbb{R}^n) = \left(\dot{H}_{p'}^1(\mathbb{R}^n)/\mathbb{R} \right)^*$, where $1/p + 1/p' = 1$.

Theorem 3.2.1 *[EPS03] Let $1 < p < \infty$, $1/p + 1/p' = 1$ and define the divergence operator*

$$\mathrm{div} : L_p(\mathbb{R}^n; \mathbb{R}^n) \to \dot{H}_p^{-1}(\mathbb{R}^n)$$

as $\mathrm{div} = -\nabla^*$ *where* $\nabla : {}_0\dot{H}_{p'}^1(\mathbb{R}^n) \to L_{p'}(\mathbb{R}^n; \mathbb{R}^n)$.

Then, div *is bounded, linear, and surjective. With $J = [0, \tau]$,* div *extends as a bounded, linear, surjective operator*

$$\mathrm{div} : H_p^1(J; L_p(\mathbb{R}^n; \mathbb{R}^n)) \to H_p^1(J; \dot{H}_p^{-1}(\mathbb{R}^n)).$$

In particular, there is a constant $C > 0$ such that for each $f \in H_p^1(J; \dot{H}_p^{-1}(\mathbb{R}^n))$ there is $\mathbf{u} \in H_p^1(J; L_p(\mathbb{R}^n; \mathbb{R}^n))$ such that $\mathrm{div}\, \mathbf{u} = f$ *and*

$$|\mathbf{u}|_{H_p^1(J; L_p(\mathbb{R}^n; \mathbb{R}^n))} \leq C \, |f|_{H_p^1(J; \dot{H}_p^{-1}(\mathbb{R}^n))}.$$

For the convenience of the reader we recall the proof which is presented in [EPS03].

Proof. Evidently, $\nabla : {}_0\dot{H}^1_p(\mathbb{R}^n) \to L_p(\mathbb{R}^n;\mathbb{R}^n)$ is bounded, linear, and injective. Therefore, its dual is bounded, linear and surjective. By definition is ${}_0\dot{H}^1_{p'}(\mathbb{R}^n)^* = H^{-1}_p(\mathbb{R}^n)$, and thereby the first assertion follows.

From reflexivity and uniform convexity of $L_p(\mathbb{R}^n)$ we infer that for each $f \in \dot{H}^{-1}_p(\mathbb{R}^n)$ there is a unique $\mathbf{u} \in L_p(\mathbb{R}^n;\mathbb{R}^n)$ with minimal norm such that $\operatorname{div}\mathbf{u} = f$. We denote by

$$R_0 : \dot{H}^{-1}_p(\mathbb{R}^n) \to L_p(\mathbb{R}^n;\mathbb{R}^n)$$

the mapping $f \mapsto \mathbf{u}$. Then, the mapping R_0 is strong-weak continuous, and there is a constant $C > 0$ such that

$$|R_0 f|_{L_p(\mathbb{R}^n;\mathbb{R}^n)} \le C\,|f|_{\dot{H}^{-1}_p(\mathbb{R}^n)} \tag{3.4}$$

holds. Given $f \in L_p(J;\dot{H}^{-1}_p(\mathbb{R}^n))$, we define $\mathbf{u}$ by means of

$$\mathbf{u}(t) = R_0 f(t), \quad t \in J.$$

Since f is Bochner-measurable and R_0 is strong-weak continuous, $\mathbf{u}$ is weakly measurable. Hence, $\mathbf{u}$ is strongly measurable by reflexivity of $L_p(\mathbb{R}^n;\mathbb{R}^n)$, due to Petti's theorem. Applying estimate (3.4) for R_0 pointwise shows that $\mathbf{u} \in L_p(J;L_p(\mathbb{R}^n;\mathbb{R}^n))$ and

$$|\mathbf{u}|_{L_p(J;L_p(\mathbb{R}^n;\mathbb{R}^n))} \le C\,|f|_{L_p(J;\dot{H}^{-1}_p(\mathbb{R}^n))}\,.$$

This result can be extended to H^1_p by setting

$$[Rf](t) = R_0 f(0) + \int_0^t R_0 \dot{f}(s)\,ds, \qquad t \in J$$

for $f \in H^1_p(J;L_p(\mathbb{R}^n))$. Then, by boundedness of div we obtain $Rf \in H^1_p(J;L_p(\mathbb{R}^n))$, and

$$|\mathbf{u}|_{H^1_p(J;L_p(\mathbb{R}^n;\mathbb{R}^n))} \le C\,|f|_{H^1_p(J;\dot{H}^{-1}_p(\mathbb{R}^n))}\,,$$

as well as $\operatorname{div} Rf(t) = f(t)$. □

We close this section with the definition of Fredholm (semi-Fredholm) operators and some remarks about. The semi-Fredholm operator comes into play at the end of subsection 3.3.3 where we have to show that the arising solution operator is not only injective, but also surjective.

Definition 3.2.5 ((Semi-)Fredholm Operator) *Let X, Y be Banach spaces. A closed linear operator $T : X \to Y$ is said to be* Fredholm *if*

(i) $N(T)$ is finite-dimensional

(ii) $R(T)$ is closed

(iii) $Y/T(X)$ *has finite-dimension, i.e.,* $T(X)$ *has finite codimension*

The index of T *is defined by*

$$\operatorname{index} T = \dim N(T) - \dim Y/T(X).$$

The operator T *is said to be* semi-Fredholm *if the conditions* (i) *and* (ii) *are satisfied.*

The main fact, which we will use, is that the property of being Fredholm (semi-Fredholm) is stable under small perturbations, i.e., the index is continuous. For this result we refer to Kato [Kat76, Chapter IV: Theorem 5.17]

3.2.1 Sectorial Operators

This section deals with the class of *sectorial operators*, i.e., with unbounded operators for which a resolvent estimate is satisfied.

Definition 3.2.6 (Sectorial Operators) *Let* X *be a complex Banach space, and* A *a closed linear operator in* X*. Then,* A *is called a* sectorial operator *if the following conditions are satisfied.*

(S1) $\overline{\mathcal{D}(A)} = X,\ \overline{R(A)} = X,\ N(A) = \{0\}$*, and* $(-\infty, 0) \subset \rho(A)$*;*

(S2) $\left|t(t+A)^{-1} \leq M\right|$ *for all* $t > 0$*, and some* $M < \infty$*.*

The class of sectorial operators in X *will be denoted by* $\mathcal{S}(X)$*.*

We denote by Σ_θ the open sector with vertex 0 and opening angle 2θ, i.e.,

$$\Sigma_\theta := \{\lambda \in \mathbb{C}\backslash\{0\} :\ |\arg\lambda| < \theta\}.$$

Assume $A \in \mathcal{S}(X)$, then by the means of Neumann series argument follows that $\Sigma_\theta \subset \rho(-A)$ for some ρ and $\sup\left\{\left|\lambda(\lambda+A)^{-1}\right| : |\arg\lambda| < \theta\right\} < \infty$. Therefore, it is reasonable to define the *spectral angle* ϕ_A of $A \in \mathcal{S}(X)$ by

$$\phi_A := \inf\left\{\phi : \Sigma_{\pi-\phi} \subset \rho(-A), \sup_{\lambda\in\Sigma_{\pi-\phi}} \left|\lambda(\lambda+A)^{-1}\right| < \infty\right\}.$$

Evidently, it holds that $\phi_A \in [0, \pi)$ and $\phi_A \geq \sup\{|\lambda| : \lambda \in \sigma(A)\}$.

In particular, we are interested in the question: for which $\lambda \in \mathbb{C}$ and $\boldsymbol{\xi} \in \mathbb{R}^n$ is $(\lambda + \mathcal{A}(\boldsymbol{\xi}))$ invertible. This leads to the assumption of ellipticity.

Definition 3.2.7 (Parameter Ellipticity) *The* $\mathcal{B}(X)$*-valued polynomial*

$$\mathcal{A}(\boldsymbol{\xi}) = \sum_{|\alpha|=m} a_\alpha \boldsymbol{\xi}^\alpha$$

is called parameter elliptic *if there is an angle* $\phi \in [0, \pi)$ *such that the spectrum* $\sigma(\mathcal{A}(\boldsymbol{\xi}))$ *of* $\mathcal{A}(\boldsymbol{\xi})$ *in* $\mathcal{B}(X)$ *satisfies*

$$\sigma(\mathcal{A}(\boldsymbol{\xi})) \subset \Sigma_\phi, \quad \text{for all } \boldsymbol{\xi} \in \mathbb{R}^n,\ |\boldsymbol{\xi}| = 1.$$

Then, we call

$$\phi_{\mathcal{A}} := \inf\{\phi : \ \sigma(\mathcal{A}(\boldsymbol{\xi})) \subset \Sigma_\phi \quad \textit{for all} \ \ \boldsymbol{\xi} \in \mathbb{R}^n, \ |\boldsymbol{\xi}| = 1\}$$

the angle of ellipticity *of* $\mathcal{A}$.

Further on, we need the stronger property of strong ellipticity.

Definition 3.2.8 (Strong Ellipticity) *The differential operator* $\mathcal{A}(\mathbf{x}, D)$ *is called* strongly elliptic*, if the numerical range of* $\mathcal{A}(\mathbf{x}, \boldsymbol{\xi})$ *is a subset of* $\{z \in \mathbb{C} : \ Re\, z > 0\}$ *for all* $\mathbf{x} \in \mathbb{R}^n$, $\boldsymbol{\xi} \in \mathbb{R}^n$ *with* $|\boldsymbol{\xi}| = 1$. *Hence, strong ellipticity means that there is a constant* $c > 0$ *such that*

$$Re\ (\mathcal{A}(\mathbf{x}, \boldsymbol{\xi})\boldsymbol{\eta}, \boldsymbol{\eta}) \geq c, \ \textit{for all} \ \boldsymbol{\xi} \in \mathbb{R}^n, \ \boldsymbol{\eta} \in \mathbb{C}^n \ \textit{with} \ |\boldsymbol{\xi}| = |\boldsymbol{\eta}| = 1, \ \mathbf{x} \in \mathbb{R}^n.$$

Let X be a Banach space, $J = [0, \tau]$ for some $\tau > 0$, and let $\mathbf{f} : J \to X$ be a function. Furthermore, let $A \in \mathcal{S}(X)$. We consider the Cauchy problem

$$\frac{\partial}{\partial t}\mathbf{u} + A\mathbf{u} = \mathbf{f}, \quad t \in J = [0, \tau], \mathbf{x} \in \mathbb{R}^n, \qquad \mathbf{u}(0) = 0 \tag{3.5}$$

in $L_p(J; X)$ for $1 < p < \infty$. Then, the definition of maximal regularity for (3.5) is as follows.

Definition 3.2.9 (Maximal L_p-regularity) *The operator* A *is said to belong to the* maximal L_p-regularity class*, if for each* $\mathbf{f} \in L_p(J; X)$ *there exists a unique* $\mathbf{u} \in H^1_p(J; X) \cap L_p(J; D_A)$ *satisfying (3.5) in the* L_p*-sense.*

Then, the closed graph theorem implies that there exists a constant $C > 0$ such that

$$\left|\frac{\partial}{\partial t}\mathbf{u}\right|_{L_p(J;X)} + |A\mathbf{u}|_{L_p(J;X)} \leq C\,|\mathbf{f}|_{L_p(J;X)}\,.$$

Maximal regularity for classes of elliptic differential operators are, e.g., studied in [KW04]. Results for elliptic problems are even known in the more general case of Banach spaces [DHP03]. Further on, in order to simplify our main proof we will use the following result for elliptic problems, which is proven by Denk, Hieber, and Prüss [DHP03]. In fact, we need this theorem in case $X = \mathbb{R}^n$ and for operators of second order.

Theorem 3.2.2 *[DHP03] Let* X *be a Banach space of class* $\mathcal{HT}$, $n, m \in \mathbb{N}$ *and* $1 < p < \infty$. *Suppose* $A(D) = \sum_{|\alpha|=m} a_\alpha D^\alpha$ *is a homogeneous differential operator of order* m *which is parameter elliptic with angle of ellipticity* $\phi_{\mathcal{A}} < \pi/2$. *Let* $\mathbf{f} \in L_p(J \times \mathbb{R}^n; X)$ *and let* A *denote its realization in* $L_p(\mathbb{R}^n; X)$ *with domain* $D(A) = H^m_p(\mathbb{R}^n; X)$. *Then the problem*

$$\frac{\partial}{\partial t}\mathbf{u} + A\mathbf{u} = \mathbf{f}, \quad t \in J = [0, \tau], \mathbf{x} \in \mathbb{R}^n, \qquad \mathbf{u}(0) = 0$$

has the property of maximal regularity in $L_p(J; L_p(\mathbb{R}^n; X))$.

3.2.2 $\mathcal{R}$-Boundedness and Fourier Multipliers

This section deals with $\mathcal{R}$-boundedness and Fourier multiplier theorems. Before we recall the scalar-version of Mikhlin's multiplier theorem and its extension to an operator-valued version, we introduce the notion of $\mathcal{R}$-bounded families of linear bounded operators. In general, $\mathcal{R}$-boundedness comes particularly into interest in connection with operator-valued multiplier theorems. For a historical overview with respect to $\mathcal{R}$-boundedness and Fourier multipliers we refer to Hytoenen [Hyt03]. Furthermore, we introduce the notion of $\mathcal{R}$-sectorial operators and recall an important theorem of Girardi and Weis [GW03] which offers a criterion in order to decide if sets of Fourier multipliers are $\mathcal{R}$-bounded. For more details about $\mathcal{R}$-boundedness and $\mathcal{R}$-sectorial we refer to the extensive work of Denk, Hieber, and Prüss [DHP03].

We start with the definition of $\mathcal{R}$-bounded families of bounded linear operators.

Definition 3.2.10 ($\mathcal{R}$-boundedness) *Let X and Y be Banach spaces. A family of operators $\mathcal{T} \subset \mathcal{B}(X,Y)$ is called $\mathcal{R}$-bounded, if there exists a constant $C > 0$ and $p \in [1,\infty)$ such that for each $N \in \mathbb{N}, T_j \in \mathcal{T}, x_j \in X$ and for all independent, symmetric, $\{-1,1\}$-valued random variables ε_j on a probability space $(\Omega, \mathcal{M}, \mu)$ the inequality*

$$\left| \sum_{j=1}^{N} \varepsilon_j T_j x_j \right|_{L_p(\Omega;Y)} \leq C \left| \sum_{j=1}^{N} \varepsilon_j x_j \right|_{L_p(\Omega;X)}$$

*is valid. The smallest C is called $\mathcal{R}$-*bound *of $\mathcal{T}$, we denote it by $\mathcal{R}(\mathcal{T})$.*

The next proposition shows that $\mathcal{R}$-bounds behave similar to norms.

Proposition 3.2.1 *[DHP03, Prop. 3.4] (a) Let X, Y be Banach spaces, and $\mathcal{T}, \mathcal{S} \subset \mathcal{B}(X,Y)$ be $\mathcal{R}$-bounded. Then*

$$\mathcal{S} + \mathcal{T} = \{S + T : S \in \mathcal{S}, T \in \mathcal{T}\}$$

is $\mathcal{R}$-bounded as well, and $\mathcal{R}\{\mathcal{S}+\mathcal{T}\} \leq \mathcal{R}\{\mathcal{S}\} + \mathcal{R}\{\mathcal{T}\}$.
(b) Let X, Y, Z be Banach spaces, and $\mathcal{T} \subset \mathcal{B}(X,Y)$ and $\mathcal{S} \subset \mathcal{B}(Y,Z)$ be $\mathcal{R}$-bounded. Then

$$\mathcal{S}\mathcal{T} = \{ST : T \in \mathcal{T}, S \in \mathcal{S}\}$$

is $\mathcal{R}$-bounded, and $\mathcal{R}(\mathcal{S}\mathcal{T}) \leq \mathcal{R}(\mathcal{S})\mathcal{R}(\mathcal{T})$.

The useful result that a holomorphic function H on a compact set K yields $\mathcal{R}$-boundedness of the family $\{H(\zeta) : \zeta \in K\}$ is stated in the following proposition.

Proposition 3.2.2 *[DHP03, Prop. 3.10] Let $G \subset \mathbb{C}$ be open, $K \subset G$ compact, and suppose $H : G \to \mathcal{B}(X,Y)$ is holomorphic. Then $H(K) \subset \mathcal{B}(X,Y)$ is $\mathcal{R}$-bounded.*

A proof of these propositions can be found in [DHP03]. The next result will be useful in section 3.3.2 and shows that an $\mathcal{R}$-bounded family can be extended in the following way.

Proposition 3.2.3 *Let $1 < p < \infty$ and $\{T(\lambda)\}_{\lambda\in\Lambda} \subset \mathcal{B}(X,Y)$ $\mathcal{R}$-bounded. Extend each $T(\lambda)$ to an operator in $\mathcal{B}(L_p(J;X), L_p(J;Y))$ by means of*

$$(T(\lambda)\mathbf{f})(t,\mathbf{x}) = (T(\lambda)\mathbf{f}(t,\cdot))(\mathbf{x}).$$

Then, the extended family is $\mathcal{R}$-bounded.

Proof. Let $N \in \mathbb{N}$, $T_j \in \{T(\lambda)\}_{\lambda\in\Lambda} \subset \mathcal{B}(X,Y)$ and $\mathbf{x}_j \in X$. Then, by definition of $\mathcal{R}$-boundedness, there is a constant C such that for all independent, symmetric, $\{-1,1\}$-valued random variables ε_j on a probability space $(\Omega,\mathcal{M},\mu)$ the inequality

$$\Big|\sum_{j=1}^{N}\varepsilon_j T_j\mathbf{x}_j\Big|_{L_p(\Omega;Y)} \le C\Big|\sum_{j=1}^{N}\varepsilon_j\mathbf{x}_j\Big|_{L_p(\Omega;X)} \tag{3.6}$$

holds. Now, we consider that T_j is an element of the extension family $\{T(\lambda)\}_{\lambda\in\Lambda} \subset \mathcal{B}(L_p(J;X),L_p(J;Y))$ and further let $\mathbf{f}_j \in L_p(J;X)$. Using Fubini's theorem and inequality (3.6) yields

$$\begin{aligned}
\Big|\sum_{j=1}^{N}\varepsilon_j T_j\mathbf{f}_j\Big|_{L_p(\Omega;L_p(J;Y))} &= \Big|\sum_{j=1}^{N}\varepsilon_j T_j\mathbf{f}_j\Big|_{L_p(J;L_p(\Omega;Y))} \\
&= \left(\int_J \Big|\sum_{j=1}^{N}\varepsilon_j T_j\mathbf{f}_j\Big|^p_{L_p(\Omega;Y)}\right)^{1/p} \\
&\le C\left(\int_J \Big|\sum_{j=1}^{N}\varepsilon_j \mathbf{f}_j\Big|^p_{L_p(\Omega;X)}\right)^{1/p} \\
&= C\Big|\sum_{j=1}^{N}\varepsilon_j \mathbf{f}_j\Big|_{L_p(J;L_p(\Omega;X))} = C\Big|\sum_{j=1}^{N}\varepsilon_j \mathbf{f}_j\Big|_{L_p(\Omega;L_p(J;X))}
\end{aligned}$$

which proves the assertion. □

We turn now to $\mathcal{R}$-sectorial operators, the definition of which is similar to the definition of sectorial operators and is basically obtained by replacing *bounded* by *$\mathcal{R}$-bounded*.

Definition 3.2.11 ($\mathcal{R}$-sectorial) *Let X be a complex Banach space and A be a sectorial operator. Then, A is called $\mathcal{R}$-sectorial if*

$$\mathcal{R}(0) := \mathcal{R}\left\{t(t+A)^{-1} :\ t>0\right\} < \infty.$$

The $\mathcal{R}$-angle ϕ_A^R of A is defined by means of

$$\phi_A^R := \inf\left\{\theta\in(0,\pi) :\ \mathcal{R}_A(\pi-\theta) < \infty\right\},$$

where

$$\mathcal{R}_A(\theta) := \mathcal{R}\left\{\lambda(\lambda + A)^{-1} : \ |\arg\lambda| \leq \theta\right\}.$$

The class of $\mathcal{R}$-sectorial operators in X will be denoted by $\mathcal{RS}(X)$.

The $\mathcal{R}$-angle of an $\mathcal{R}$-sectorial operator A is well-defined and is not smaller than the spectral angle of A, [DHP03, Definition 4.1]. In [CP01], Clèment and Prüss prove that the class of operators with bounded imaginary powers ($BIP(X)$) is contained in the class of $\mathcal{R}$-sectorial operators, provided that the underlying Banach space X belongs to the class $\mathcal{HT}$. We recall the definition of the class $\mathcal{HT}$.

Definition 3.2.12 (Class $\mathcal{HT}$) *A Banach space X belongs to the class $\mathcal{HT}$ if the Hilbert transform is bounded on $L_p(\mathbb{R}, X)$ for some (and then all) $1 < p < \infty$. The* Hilbert transform H *of a function $f \in S(\mathbb{R}; X)$ is defined by*

$$(Hf)(x) := \frac{1}{\pi} \lim_{\varepsilon \to 0} \int_{\varepsilon \leq |s| \leq 1/\varepsilon} \frac{f(t-s)}{s}\, ds, \qquad t \in \mathbb{R},$$

where the limit is to be understood in the L_p-sense.

It is known that the $\mathcal{HT}$-spaces are reflexive and the set of Banach spaces of class $\mathcal{HT}$ coincides with the class of UMD-spaces, where UMD stands for *unconditional martingale difference property*. Each Hilbert space belongs to the class $\mathcal{HT}$. If $(\Omega, \mathcal{A}, \mu)$ is a measure space, $1 < p < \infty$, then $L_p(\Omega, \mathcal{A}, \mu; X)$ is an $\mathcal{HT}$-space provided that X is of class $\mathcal{HT}$. For these and related results see [Bur86], [Prü93].

Before we turn to some criteria given in [GW03] in order to decide if a set of Fourier multipliers is $\mathcal{R}$-bounded, we recall the classical Mikhlin multiplier theorem in n dimensions.

The space $\mathcal{D}(\mathbb{R}^n; \mathbb{R}^n)$ denotes the space of all C^∞-functions with compact support on $\mathbb{R}^n$ equipped with the topology that is given by the usual family of semi-norms [Yos80]. Let $\mathcal{D}'(\mathbb{R}^n; \mathbb{R}^n) := \mathcal{B}(\mathcal{D}(\mathbb{R}^n), \mathbb{R}^n)$ be the space of distributions. The *Schwartz space* $S(\mathbb{R}^n; \mathbb{R}^n)$ consists of all infinitely differentiable, rapidly decreasing functions. The tempered distributions are defined by $S'(\mathbb{R}^n; \mathbb{R}^n) := \mathcal{B}(S(\mathbb{R}^n), \mathbb{R}^n)$. Then, given $\mathcal{M} \in L_{1,\mathrm{loc}}(\mathbb{R}^n; \mathcal{B}(\mathbb{R}^n))$, we may define an operator $T_{\mathcal{M}} : \mathcal{F}^{-1}\mathcal{D}(\mathbb{R}^n; \mathbb{R}^n) \to \mathcal{S}'(\mathbb{R}^n; \mathbb{R}^n)$ by means of

$$T_{\mathcal{M}}\phi := \mathcal{F}^{-1}\mathcal{M}\mathcal{F}\phi, \qquad \text{for all } \mathcal{F}\phi \in \mathcal{D}(\mathbb{R}^n; \mathbb{R}^n).$$

Since $\mathcal{F}^{-1}\mathcal{D}(\mathbb{R}^n; \mathbb{R}^n)$ is dense in $L_p(\mathbb{R}^n; \mathbb{R}^n)$, the operator T_M is well-defined and linear on a dense subspace of $L_p(\mathbb{R}^n; \mathbb{R}^n)$.

The question arises: on which assumptions on the multiplier $\mathcal{M}$ is the operator $T_{\mathcal{M}}$ bounded in L_p.

Theorem 3.2.3 (Mikhlin Fourier Multiplier in $\mathbb{R}^n$) *Let $1 < p < \infty$. Assume that $\mathcal{M} \in \mathcal{C}^L(\mathbb{R}^n \backslash \{0\}; \mathbb{R}^n)$ satisfies*

$$K := \sup\{|\boldsymbol{\xi}|^{|\alpha|}\, D^\alpha \mathcal{M}(\boldsymbol{\xi})\} < \infty \qquad \forall \alpha \in \{0,1\}^n, |\alpha| \leq L \text{ and } \boldsymbol{\xi} \in \mathbb{R}^n \backslash \{0\} \tag{3.7}$$

where L is an integer with $L > \frac{n}{2}$. Then the operator T_M defined by

$$T_{\mathcal{M}}\phi := \mathcal{F}^{-1}\mathcal{M}\mathcal{F}\phi, \qquad \text{for all } \mathcal{F}\phi \in \mathcal{D}(\mathbb{R}^n;\mathbb{R}^n)$$

is bounded from $L_p(\mathbb{R}^n;\mathbb{R}^n)$ into $L_p(\mathbb{R}^n;\mathbb{R}^n)$ with norm

$$|T_{\mathcal{M}}|_{\mathcal{B}(L_p(\mathbb{R}^n;\mathbb{R}^n))} \leq C\ K,$$

where C depends on p and n.

A proof of this theorem can be found in [BL76, Section 6.1].

A large class of multipliers are Calderón-Zygmund operators, i.e., convolution operators with singular integral kernels, see for example [Duo01], [Ste98]. If $\mathcal{M}$ is a symbol of order 0, then $T_{\mathcal{M}}$ is a Calderón-Zygmund operator and Calderón-Zygmund operator are L_p-bounded [Duo01].

The Mikhlin multiplier theorem can be extended to the operator-valued case in one dimension as well as in n dimensions. In the one dimensional case this was first shown by Weis [Wei01] using the concept of $\mathcal{R}$-boundedness. In general, the condition (3.7) has to be replaced by $\mathcal{R}$-boundedness. In [CP01], Clément and Prüss have shown that $\mathcal{R}$-boundedness of the family $\{\mathcal{M}(\rho) :\ \rho \text{ is Lebesgue point of } \mathcal{M}\}$ is necessary. Results about the operator-valued case in one-dimension as well as in n dimensions can be found, e.g., in [DHP03], [KW04]. A comparison of multipliers on Besov and Bochner spaces as well as a detailed survey of the historical development of multipliers is given in [Hyt03].

We close this section with the announced theorem of Girardi and Weis. Before, we recall that a Banach space X has *Fourier type* q, where $q \in [1,2]$, if the Fourier transform defines a bounded operator from $L_q(X)$ into $L_{q'}(X)$, i.e., the Hausdorff Young inequality

$$|\mathcal{F}f|_{L_{q'}(X)} \leq C\,|f|_{L_q(X)}$$

holds. Since each Banach space has Fourier type 1, the case $q > 1$ is also called *non-trivial Fourier type q*. For a definition property (α) we refer to [Hyt03]. We mention that each L_p-space has property (α).

Theorem 3.2.4 *[GW03, Theorem 3.2] Let X and Y be UMD Banach spaces having property (α) and Fourier type q. Let $l = [n/q] + 1$. Let τ be a $\mathcal{R}$-bounded subset of $\mathcal{B}(X;Y)$ and*

$$\mathcal{M}^l(\tau) := \Big\{M : \mathbb{R}^n\backslash\{0\} \to \mathcal{B}(X;Y) :\ |\boldsymbol{\xi}|^{|\alpha|}\, D^\alpha M(\boldsymbol{\xi}) \in \tau \text{ for } \boldsymbol{\xi} \in \mathbb{R}^n\backslash\{0\},\ \alpha \in \mathbb{N}_0^n,\ |\alpha| \leq l\Big\}.$$

Then the set of Fourier multiplier operators

$$\Big\{T_M \in \mathcal{B}(L_p(\mathbb{R}^n;X), L_p(\mathbb{R}^n;Y)) :\ M \in \mathcal{M}^l(\tau)\Big\}$$

is $\mathcal{R}$-bounded.

3.2.3 $\mathcal{H}^\infty$-calculus

In order to achieve that the solution of system (3.2) is in the maximal L_p-regularity class, we need a result of Kalton and Weis [KW01] on the existence of an operator-valued functional calculus for operators with an $\mathcal{H}^\infty$-calculus. As preparation, we consider first the concept of the $\mathcal{H}^\infty$-calculus where we follow the paper of Denk, Hieber, and Prüss [DHP03] and show that the time derivative operator on $\mathbb{R}$ admits a bounded $\mathcal{H}^\infty$-calculus in L_p. Finally, we recall a result about sums of closed operators of of Kalton and Weis [KW01] and recall the so-called mixed derivative theorem.

For $\phi \in (0, \pi]$, we define by $\mathcal{H}(\Sigma_\phi)$ the algebra of all holomorphic functions on Σ_ϕ, hence

$$\mathcal{H}(\Sigma_\phi) := \{f : \Sigma_\phi \to \mathbb{C} \text{ holomorphic}\},$$

and let

$$\mathcal{H}^\infty(\Sigma_\phi) := \{f : \Sigma_\phi \to \mathbb{C} \text{ holomorphic and bounded}\},$$

which when equipped with norm $|f|_\infty^\phi := \sup_{\lambda\in\Sigma_\phi} |f(\lambda)|$ is a Banach algebra. Further, we define the subspace

$$\mathcal{H}_0(\Sigma_\phi) = \bigcup_{\alpha,\beta<0} \mathcal{H}_{\alpha,\beta}(\Sigma_\phi) \text{ where } \mathcal{H}_{\alpha,\beta}(\Sigma_\phi) := \left\{ f \in \mathcal{H}(\Sigma_\phi) : |f|_{\alpha,\beta}^\phi < \infty \right\}$$

endowed with the norm $|f|_{\alpha,\beta}^\phi := \sup_{|\lambda|\le 1} |\lambda^\alpha f(\lambda)| + \sup_{|\lambda|\ge 1} \left|\lambda^{-\beta} f(\lambda)\right|$.

Let A be a sectorial operator and fix any $\psi \in (\phi_A, \pi]$. We define by Γ_ψ the oriented integration path $\Gamma_\psi = |t|\ e^{-i\,\mathrm{sign}(t)\psi},\ t \in \mathbb{R}$. Then, the Dunford integral

$$f(A) = \frac{1}{2\pi i} \int_{\Gamma_\psi} f(\lambda)\,(\lambda - A)^{-1}\ d\lambda, \qquad f \in \mathcal{H}_0(\Sigma_\phi)$$

defines via $\Phi_A(f) = f(A)$ a functional calculus $\Phi : \mathcal{H}_0(\Sigma_\phi) \to \mathcal{B}(X)$ which is a bounded algebra homomorphism.

Definition 3.2.13 *A sectorial operator A in X admits a bounded $\mathcal{H}^\infty$-calculus if there are $\phi > \phi_A$ and a constant $K_\phi < \infty$ such that*

$$|f(A)| \le K_\phi\, |f|_\infty^\phi, \qquad \text{for all } f \in \mathcal{H}_0(\Sigma_\phi). \tag{3.8}$$

The class of sectorial operators A which admit an $\mathcal{H}^\infty$-calculus will be denoted by $\mathcal{H}^\infty(X)$. The $\mathcal{H}^\infty$-angle of A is defined by

$$\phi_A^\infty := \inf\{\phi > \phi_A : (3.8) \textit{is valid}\}.$$

In the case that $A \in \mathcal{H}^\infty(X)$, the functional calculus for A on $\mathcal{H}_0(\Sigma_\phi)$ extends uniquely to $\mathcal{H}^\infty(\Sigma_\phi)$.

For the spaces $\mathcal{S}(X)$, $\mathcal{RS}(X)$, $BIP(X)$ and $\mathcal{H}^\infty(X)$ we have

$$\mathcal{H}^\infty(X) \subseteq BIP(X) \subseteq \mathcal{RS}(X) \subseteq \mathcal{S}(X)$$

with the corresponding angles $\phi_A^\infty \geq \theta_A \geq \phi_A^R \geq \phi_A$ (see [DHP03]).

Next, we show that the time derivative operator d/dt admits an $\mathcal{H}^\infty$-calculus [KW04].

Proposition 3.2.4 *Let X be a Banach space of class $\mathcal{HT}$ and $B = d/dt$ on $Y := L_p(\mathbb{R}; X)$ with $1 < p < \infty$. Then, $B \in \mathcal{H}^\infty(Y)$ with $\mathcal{H}^\infty$-angle $\phi_B^\infty = \pi/2$.*

Proof. Let $\phi < \pi/2$ be fixed and choose a function $h \in \mathcal{H}_0(\Sigma_\phi)$. Further, let Γ_θ be the contour $\Gamma_\theta = |t|\, e^{i\ \mathrm{sign}(t)\theta}$, $t \in \mathbb{R}$, where $\phi < \theta < \pi/2$. Then, $h(B)$ is well-defined as Dunford integral

$$h(B) = \frac{1}{2\pi i} \int_{\Gamma_\theta} h(\lambda)(\lambda - B)^{-1}\, d\lambda.$$

For $g \in S(\mathbb{R}; X)$, we take the Fourier transform

$$\begin{aligned} \mathcal{F}[h(B)g](\rho) &= \frac{1}{2\pi i} \int_{\Gamma_\theta} h(\lambda)(\lambda - i\rho)^{-1} (\mathcal{F}g)(i\rho)\, d\lambda \\ &= h(i\rho)(\mathcal{F}g)(\rho). \end{aligned}$$

Thus, the symbol of $h(B)$ is given by $h(i\rho)$. Therefore, it remains to show that $h(i\rho)$ is a Fourier multiplier. In order to apply Mikhlin multiplier theorem 3.2.3 with $n = 1$, it is sufficient to show that $|h(i\rho)|$ and $|\rho\, h'(i\rho)|$ for $\rho \in \mathbb{R}\backslash\{0\}$ are bounded. For $\lambda \in \Gamma_\theta$ and $\rho \in \mathbb{R}\backslash\{0\}$, we obtain

$$\rho\, h'(i\rho) = \frac{1}{2\pi i} \int_{\Gamma_\theta} \frac{\rho}{(\lambda - i\rho)^2} h(\lambda)\, d\lambda$$

Due to uniformly boundedness of the integrand in $L_1(\Gamma_\theta)$, $\phi < \theta < \pi/2$, we get

$$\sup_{\rho \in \mathbb{R}} |h(i\rho)| \leq \sup_{\mu \in \Sigma_\phi} |h(\mu)| \leq |h|_\phi^\infty$$

and

$$\sup_{\rho \in \mathbb{R}} \left|\rho\, h'(i\rho)\right| \leq C \sup_{\mu \in \Sigma_\phi} |h(\mu)| \leq C\, |h|_\phi^\infty\,.$$

Hence, the functional calculus $\Phi_B(h) = h(B)$ defines a bounded operator on $L_p(\mathbb{R}; X)$. □

Before we quote the next result, we recall that two closed linear operators A, B in X are said to *commute in the resolvent sense*, if there exist $\lambda \in \rho(A)$ and $\mu \in \rho(B)$ such that

$$(\lambda - A)^{-1}(\mu - B)^{-1} = (\mu - B)^{-1}(\lambda - A)^{-1}.$$

Theorem 3.2.5 *[KW01, Theorem 4.4] Let X be a Banach space. Let A and F be sectorial operators in X commuting in the resolvent sense. Suppose that A admits an $\mathcal{H}^\infty(\Sigma_\phi)$-calculus and $F \in \mathcal{H}^\infty(\Sigma_\sigma; \mathcal{B}(X))$ for some $\sigma > \phi$. Suppose further that the set $\{F(\mu) : \mu \in \Sigma_\sigma\}$ is $\mathcal{R}$-bounded. Then, $F(A) \in \mathcal{B}(X)$.*

In the following, we are interested in the sum of closed linear operators A, B in X [Prü93, Section 8.3]. Let $A + B$ be defined by

$$(A + B)x = Ax + Bx, \qquad x \in D(A + B) := D(A) \cap D(B).$$

If $0 \in \rho(A + B)$, which implies that $(A + B)$ is closed, then the solution x of

$$Ax + Bx = y \tag{3.9}$$

belongs to $D(A) \cap D(B)$ for all $y \in X$. Thus, the solution x has *maximal regularity*. Application of the closed graph theorem leads to the estimate

$$|Ax| + |Bx| \leq C\,|Ax + Bx| \qquad \text{for all } x \in D(A + B).$$

If $A + B$ is closable, but not closed, and $0 \in \rho(\overline{A + B})$ then problem (3.9) only admits generalized solutions in the sense that there are sequences $(x_n) \subset D(A) \cap D(B), x_n \to x$, and $y_n \to y$ satisfying

$$Ax_n + Bx_n = y_n, \quad n \in \mathbb{N}.$$

In general, nothing can be said about $A + B$, it need not even be closable, unless further assumptions on A and B are imposed.

The following fundamental result was shown by Da Prato and Grisvard [DG75]. If A and B are sectorial operators commuting in the resolvent sense and satisfy the parabolicity condition $\phi_A + \phi_B < \pi$, the sum $A + B$ is closable and the closure $L := \overline{A + B}$ of $A + B$ with $D(A + B) = D(A) \cap D(B)$ is sectorial with $\phi_L \leq \max\{\phi_A, \phi_B\}$.

However, the result that the sum $A + B$ is already closed on $D(A) \cap D(B)$ is often needed. In [DV87], Dore and Venni showed closedness of $A + B$ provided that A and B are operators of bounded imaginary powers and the underlying Banach space X is of class $\mathcal{HT}$. Monniaux and Prüss extended this Dore-Venni theorem to the case where the operators are non-commuting but instead satisfy a certain commutator condition [MP97].

Without restriction on the underlying Banach space X, but strengthening the assumption for one operator, Kalton and Weis [KW01] showed the following criterion in order to achieve closedness of $A + B$.

Theorem 3.2.6 *[KW01, Theorem 6.3] Let X be a Banach space. Let A and B be sectorial operators commuting in the resolvent sense. Assume that the operator A admits an H^∞-calculus and B is $\mathcal{R}$-sectorial. Furthermore, suppose that the parabolicity condition $\phi_A^\infty + \phi_B^R < \pi$ is satisfied. Then, $A + B$ is closed on the domain $D(A) \cap D(B)$ and there is a constant C such that*

$$|Ax| + |Bx| \leq C\,|Ax + Bx|\,, \qquad x \in D(A) \cap D(B).$$

In connection with the method of sums, we recall the so-called *mixed derivative theorem* which goes back to Sobolevskii.

Theorem 3.2.7 (Mixed Derivative Theorem) *[Prü93] Suppose A, B are sectorial operators in a Banach space X which commute in the resolvent sense and their spectral angles satisfy the parabolicity condition $\phi_A + \phi_B < \pi$. Furthermore, we assume that the pair (A, B) is coercively positive, i.e., $A + \mu B$ with natural domain $D(A + \mu B) = D(A) \cap D(B)$ is closed for each $\mu > 0$ and there is a constant $M > 0$ such that*

$$|Ax|_X + |\mu Bx|_X \leq M \, |Ax + \mu Bx|_X \qquad \text{for all } x \in D(A) \cap D(B),\ \mu > 0.$$

Then, there exists a constant $C > 0$ such that

$$\left|A^{\alpha} B^{1-\alpha} x\right|_X \leq C \, |Ax + \mu Bx|_X \qquad \text{for all } x \in D(A) \cap D(B), \quad \alpha \in [0, 1].$$

For additional results concerning complex and real interpolation we refer to [BL76], [Tri92]. We close this section with an embedding result, e.g. [Kot03], which will be used in section 3.3.4.

Proposition 3.2.5 *Let $1 < p < \infty$, fix a time interval $J_0 = [0, \tau_0]$ and let $J = [0, \tau]$ for $\tau \leq \tau_0$. Set*

$$Z_\tau := H_p^1(J_\tau; L_p(\mathbb{R}^n; \mathbb{R}^n)) \cap L_p(J_\tau; H_p^2(\mathbb{R}^n; \mathbb{R}^n))$$

and

$$X_p := W_p^{2-2/p}(\mathbb{R}^n; \mathbb{R}^n)$$

for the time-trace space of Z_τ. Furthermore, we define

$${}_0Z_\tau := \left\{ \mathbf{u} \in Z_\tau : \mathbf{u}_{|_{t=0}} = 0 \right\}$$

if the trace exists. Then, the embedding

$${}_0Z_\tau \hookrightarrow C(J_\tau; X_p)$$

is valid and the embedding constant is uniform with respect to $\tau \in (0, \tau_0]$.

Proof. By the mixed derivative theorem 3.2.7, we obtain

$$Z_\tau \hookrightarrow H_p^\theta(J_\tau; H^{2(1-\theta)}(\mathbb{R}^n; \mathbb{R}^n)) \qquad \text{for } 0 < \theta < 1.$$

Thus, for the time-trace space the desired embedding of Z_τ

$${}_0Z_\tau \hookrightarrow C(J_\tau; X_p)$$

is valid. In order to show that the embedding constant is uniform, we define the extension operator E_+ as

$$E_+\mathbf{u} = \begin{cases} \mathbf{u}(t,\mathbf{x}) & : \ t \in [0,\tau) \\ \mathbf{u}(2\tau - t,\mathbf{x}) & : \ t \in [\tau, 2\tau) \\ 0 & : \ t \in [2\tau,\infty). \end{cases}$$

for $\mathbf{u} \in {}_0Z_\tau$. Observe that E_+ is a bounded operator with norm $|E_+|_{\mathcal{B}({}_0Z_\tau,{}_0Z(\mathbb{R}^+))} \leq 2$, where ${}_0Z(\mathbb{R}^+)$ corresponds to ${}_0Z_\tau$ with $J_\tau = \mathbb{R}^+$. Thus, we obtain the estimate

$$\begin{aligned} |\mathbf{u}(t,\mathbf{x})|_{C(J_\tau;X_p)} &\leq |E_+\mathbf{u}|_{C(\mathbb{R}_+;X_p)} \\ &\leq M\,|E_+\mathbf{u}|_{{}_0Z(\mathbb{R}^+)} \\ &\leq 2\,M\,|\mathbf{u}|_{{}_0Z_\tau} \end{aligned}$$

where the constant M results from the embedding for $J_\tau = \mathbb{R}_+$ and as a result of this, M is independent of the time interval length τ. □

3.3 Existence Result for Generalized Newtonian Flows

In this section we formulate the main theoretical result of this thesis. By means of maximal L_p-regularity, we show local (in time) strong well-posedness of model (3.2) under certain restrictions concerning the viscosity function $\mu(\|\mathbf{D}\|^2)$. Previous to that, using a closer examination of the term $\operatorname{div}\mathbf{S}$, we reformulate system (3.2) such that we achieve an abstract but equivalent formulation which is given in theorem 3.3.1.

We consider the viscous stress tensor $\mathbf{S} = 2\mu(\|\mathbf{D}\|^2)\mathbf{D}$ with $\mathbf{D} = (d_{ij})_{i,j=1,\dots,n}$. Then, the i^{th} entry of $\operatorname{div}\mathbf{S}$ can be written as follows

$$\begin{aligned} \Big[\operatorname{div}\Big(2\ \mu(\|\mathbf{D}\|^2)\mathbf{D}\Big)\Big]_i &= \sum_{j=1}^{n} \partial_j \Big(2\ \mu(\|\mathbf{D}\|^2)\ d_{ji}\Big) \\ &= \mu(\|\mathbf{D}\|^2)\sum_{j=1}^{n}\partial_j(\partial_j u_i + \partial_i u_j) + 2\ \mu'(\|\mathbf{D}\|^2)\sum_{j=1}^{n} d_{ji}\ \partial_j\,\|\mathbf{D}\|^2 \end{aligned}$$

with $\partial_j\,\|\mathbf{D}\|^2 = 2\sum_{k,l=1}^{n} d_{kl}\ \partial_j d_{kl}$. Using symmetry of $\mathbf{D}$ we obtain

$$\Big[\operatorname{div}\Big(2\ \mu(\|\mathbf{D}\|^2)\mathbf{D}\Big)\Big]_i = \mu(\|\mathbf{D}\|^2)\,(\Delta u_i + \partial_i \operatorname{div}\mathbf{u}) + 4\mu'(\|\mathbf{D}\|^2)\ \sum_{j,k,l} d_{ik}\ d_{jl}\ \partial_k\partial_l u_j$$

which reduces to

$$\Big[\operatorname{div}\Big(2\ \mu(\|\mathbf{D}\|^2)\mathbf{D}\Big)\Big]_i = \mu(\|\mathbf{D}\|^2)\Delta u_i + 4\mu'(\|\mathbf{D}\|^2)\sum_{j,k,l}^{n} d_{ik}\ d_{jl}\ \partial_k\partial_l u_j$$

in case of divergence-free velocity $\mathbf{u}$. Define the quasi-linear differential operator $\mathcal{A}(\mathbf{u}, D)$ as

$$\mathcal{A}(\mathbf{u}, D) = \sum_{k,l} A^{k,l}(\mathbf{u}) D_k D_l \tag{3.10}$$

with $D_k = -i\,\partial_k$ and the matrix-valued coefficients

$$A^{k,l}(\mathbf{u}) = \left(a^{k,l}_{i,j}(\mathbf{u})\right), \quad a^{k,l}_{i,j}(\mathbf{u}) = \mu(\|\mathbf{D}\|^2)\,\delta_{kl}\,\delta_{ij} + 4\mu'(\|\mathbf{D}\|^2)\,d_{ik}(\mathbf{u})\,d_{jl}(\mathbf{u}) \tag{3.11}$$

where δ_{kl} denotes the Kronecker symbol. Observe that, if $\mathbf{u} \in W_p^{2-2/p}(\mathbb{R}^n;\mathbb{R}^n)$ is given and $p > n+2$, then by the Sobolev embedding

$$W_p^{2-2/p}(\mathbb{R}^n;\mathbb{R}^n) \hookrightarrow BUC^1(\mathbb{R}^n;\mathbb{R}^n)$$

the coefficients of the differential operator $\mathcal{A}(\mathbf{x}, D)$, which results from inserting $\mathbf{u}$ in (3.10), are uniformly continuous. Furthermore, due to $|\nabla\mathbf{u}(\mathbf{x})| \to 0$ as $|\mathbf{x}| \to \infty$, these coefficients have a limit as $|\mathbf{x}| \to \infty$ which corresponds to the differential operator

$$\mathcal{A}(\infty, D)\mathbf{u} = -\mu(0)\Delta\mathbf{u}.$$

With this notations, problem (3.2) can be rewritten as

$$\begin{array}{rcll} \frac{\partial}{\partial t}\mathbf{u} + \mathcal{A}(\mathbf{u}, D)\mathbf{u} + \nabla p &=& F(t, \mathbf{x}, \mathbf{u}, \nabla\mathbf{u}) & \text{in } J \times \mathbb{R}^n \\ \operatorname{div}\mathbf{u} &=& 0 & \text{in } J \times \mathbb{R}^n \\ \mathbf{u}_{|_{t=0}} &=& \mathbf{u}_0 & \text{in } \mathbb{R}^n, \end{array} \tag{3.12}$$

where the nonlinearity F is given by

$$F(t, \mathbf{x}, \mathbf{u}, \nabla\mathbf{u}) = \mathbf{f}(t, \mathbf{x}) - \mathbf{u} \cdot \nabla\mathbf{u}.$$

Now, the main result reads as follows.

Theorem 3.3.1 *Let $n \in \mathbb{N}, n > 1$ and fix $p > n+2$. Let the viscosity function μ belong to $C^2(\mathbb{R}_+)$ such that*

$$\mu(s) > 0 \quad \text{and} \quad \mu(s) + 4\left(1 - \frac{1}{n}\right) s\,\mu'(s) > 0 \quad \text{for all} \quad s \geq 0.$$

Then, for each initial value $\mathbf{u}_0 \in W_p^{2-2/p}(\mathbb{R}^n;\mathbb{R}^n)$ with $\operatorname{div}\mathbf{u}_0 = 0$, there is $\tau > 0$ and a unique solution $(\mathbf{u}, p)$ of system (3.12) on $J = [0, \tau]$ within the maximal regularity class, i.e.,

$$\mathbf{u} \in H_p^1(J; L_p(\mathbb{R}^n;\mathbb{R}^n)) \cap L_p(J; H_p^2(\mathbb{R}^n;\mathbb{R}^n)), \qquad \nabla p \in L_p(J \times \mathbb{R}^n;\mathbb{R}^n).$$

The proof of this theorem is divided into several parts, which are given in the following subsections.

3.3.1 Strong Ellipticity

We consider the pseudo-differential operator $\mathcal{A}(\mathbf{x}, D)$, corresponding to (3.10), which acts on $\mathbb{R}^n$-valued functions as

$$\mathcal{A}(\mathbf{x}, D)\mathbf{v}(\mathbf{x}) = \sum_{k,l=1}^{n} A^{k,l}(\mathbf{x})\ D_k D_l \mathbf{v}(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^n. \tag{3.13}$$

Its symbol is given by the matrix

$$\mathcal{A}(\mathbf{x}, \boldsymbol{\xi}) = \sum_{k,l=1}^{n} A^{k,l}(\mathbf{x})\ \xi_k \xi_l, \qquad \mathbf{x}, \boldsymbol{\xi} \in \mathbb{R}^n.$$

The next result clarifies what the condition of strongly ellipticity means in the case that the $A^{k,l}$ stem from (3.11) with $\mathbf{u} \in W_p^{2-2/p}(\mathbb{R}^n; \mathbb{R}^n)$.

Lemma 3.3.1 *Let $n \in \mathbb{N}$, $n > 1$. Let $\mathcal{A}(\mathbf{x}, D)$ be given by (3.13) where the matrices $A^{k,l}$ are defined by (3.11) for a fixed $\mathbf{u} \in W_p^{2-2/p}(\mathbb{R}^n; \mathbb{R}^n)$ and with $\mu \in C^2(\mathbb{R}_+)$. Then, $\mathcal{A}(\mathbf{x}, D)$ is strongly elliptic, provided that*

$$\mu(s) > 0 \quad \text{and} \quad \mu(s) + 4\left(1 - \frac{1}{n}\right) s\ \mu'(s) > 0 \quad \text{for all} \quad s \geq 0.$$

Proof. Let $\mathbf{x} \in \mathbb{R}^n,\ \boldsymbol{\xi} \in \mathbb{R}^n,\ \boldsymbol{\eta} \in \mathbb{C}^n$ with $|\boldsymbol{\xi}| = |\boldsymbol{\eta}| = 1$. Referring to definition 3.2.8, we consider

$$(\mathcal{A}(\mathbf{x}, \boldsymbol{\xi})\boldsymbol{\eta}, \boldsymbol{\eta}) = \sum_{i,j,k,l}^{n} a_{i,j}^{k,l}\ \xi_k\ \xi_l\ \eta_i\ \overline{\eta}_j$$

and insert the matrices $\left(a_{i,j}^{k,l}\right)$ from equation (3.11) such that we obtain

$$\begin{aligned}
(\mathcal{A}(\mathbf{x}, \boldsymbol{\xi})\boldsymbol{\eta}, \boldsymbol{\eta}) &= \mu \sum_{i,k=1}^{n} \xi_k^2\ \eta_i\ \overline{\eta}_i + \ 4\ \mu' \sum_{i,k=1}^{n} d_{ik}\ \xi_k\ \eta_i \sum_{j,l}^{n} d_{jl}\ \xi_l\ \overline{\eta}_j \\
&= \mu\ |\boldsymbol{\xi}|^2\ |\boldsymbol{\eta}|^2 + \ 4\ \mu'\ (\mathbf{D}\boldsymbol{\xi}, \boldsymbol{\eta})\ \overline{(\mathbf{D}\boldsymbol{\xi}, \boldsymbol{\eta})} \\
&= \mu\ |\boldsymbol{\xi}|^2\ |\boldsymbol{\eta}|^2 + \ 4\ \mu'\ |(\mathbf{D}\boldsymbol{\xi}, \boldsymbol{\eta})|^2\,,
\end{aligned} \tag{3.14}$$

where $\mu := \mu(\|\mathbf{D}(\mathbf{x})\|^2)$ and $\mu' := \mu'(\|\mathbf{D}(\mathbf{x})\|^2)$. In particular, we have that $(\mathcal{A}(\mathbf{x}, \boldsymbol{\xi})\boldsymbol{\eta}, \boldsymbol{\eta})$ is real. Evidently, the operator $A(\mathbf{x}, D)$ is strongly elliptic, if $\mu > 0$ and $\mu' \geq 0$. In the case that $\mu > 0$ and $\mu' < 0$ holds, we infer from the Cauchy-Schwarz inequality

$$\text{Re}\ (\mathcal{A}(\mathbf{x}, \boldsymbol{\xi})\boldsymbol{\eta}, \boldsymbol{\eta}) \geq \mu(\|\mathbf{D}(\mathbf{x})\|^2) + 4\ \mu'(\|\mathbf{D}(\mathbf{x})\|^2)\ \|\mathbf{D}(\mathbf{x})\|^2$$

due to $|\boldsymbol{\xi}| = |\boldsymbol{\eta}| = 1$. Thus, the stronger condition

$$\mu(s) > 0 \quad \text{and} \quad \mu(s) + 4\, s\, \mu'(s) > 0 \quad \text{for } s \geq 0 \tag{3.15}$$

is sufficient. In order to improve estimate (3.15), we use the condition $\operatorname{tr} \mathbf{D} = 0$ which is equivalent to the divergence-free condition.

Since the deformation tensor $\mathbf{D}$ is symmetric and real, there is $\mathbf{S} \in \mathbb{R}^{n\times n}$ with $\mathbf{S}\mathbf{S}^T = \mathbf{I}$ such that $\boldsymbol{\Lambda} = \mathbf{S}^T\mathbf{D}(\mathbf{x})\mathbf{S}$ is a diagonal matrix, i.e., $\boldsymbol{\Lambda} = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$ where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of $\mathbf{D}(\mathbf{x})$. Thus, the term in equation (3.14) can be estimated as

$$|(\mathbf{D}(\mathbf{x})\boldsymbol{\xi}, \boldsymbol{\eta})|^2 \leq \|\mathbf{D}(\mathbf{x})\boldsymbol{\xi}\|^2 = \left(\mathbf{S}\boldsymbol{\Lambda}\mathbf{S}^T\boldsymbol{\xi}, \mathbf{S}\boldsymbol{\Lambda}\mathbf{S}^T\boldsymbol{\xi}\right) = \left\|\boldsymbol{\Lambda}\mathbf{S}^T\boldsymbol{\xi}\right\|^2$$

and we obtain

$$\begin{aligned}
\max\left\{|(\mathbf{D}(\mathbf{x})\boldsymbol{\xi}, \boldsymbol{\eta})|^2 :\ |\boldsymbol{\xi}| = |\boldsymbol{\eta}| = 1\right\} &\leq \max_{|\boldsymbol{\xi}|=1} \left\|\boldsymbol{\Lambda}\mathbf{S}^T\boldsymbol{\xi}\right\|^2 \\
&= \max\left\{\sum_{i=1}^n \lambda_i^2 y_i^2 :\ \|\mathbf{y}\| = 1\right\} \\
&= \max_{i=1,\ldots,n} |\lambda_i|^2 .
\end{aligned}$$

Therefore, searching for a better estimate than (3.15) means to find a constant $c > 0$ such that

$$\max_{i=1,\ldots,n} |\lambda_i|^2 \leq c \sum_{i=1}^n \lambda_i^2 = c\,\|\mathbf{D}\|^2 \qquad \forall\, \lambda_i \in \mathbb{R} \text{ with } \operatorname{tr}\mathbf{D} = \sum_{i=1}^n \lambda_i = 0 \tag{3.16}$$

holds. We assume that λ_1 is the eigenvalue of largest absolute value. In the case that $\lambda_1 = 0$, the inequality (3.16) becomes equality for arbitrary c. Additionally, both the inequality and the side condition (3.16) are invariant with respect to the sign of λ_i for all $i = 1, \ldots, n$. Hence, we may assume w.l.o.g that $\lambda_1 > 0$ and divide inequality (3.16) by λ_1. Let $x_i := \lambda_i/\lambda_1$ such that for $n > 1$ follows

$$\frac{1}{c} \leq 1 + \sum_{i=2}^n x_i^2. \tag{3.17}$$

From the side condition $\sum_{i=1}^n \lambda_i = 0$ we get $\sum_{i=2}^n x_i = -1$. Usage of Lagrange-Multipliers yields the function

$$f(\mathbf{x}, \sigma) = \left(1 + \sum_{i=2}^n x_i^2\right) + \sigma\left(1 + \sum_{i=2}^n x_i\right).$$

By differentiating f we obtain $\frac{\partial f}{\partial x_i} = 2x_i + \sigma \stackrel{!}{=} 0$ and $\frac{\partial f}{\partial \sigma} = 1 + \sum_{i=2}^n x_i \stackrel{!}{=} 0$. Thus, short computation results in $x_i = -\sigma/2$ and $\sigma = \frac{2}{n-1}$. From inequality (3.17) we infer that

$$c = 1 - \frac{1}{n}. \tag{3.18}$$

Combining (3.14), (3.16), and (3.18) results in

$$\text{Re } (\mathcal{A}(\mathbf{x},\boldsymbol{\xi})\boldsymbol{\eta},\boldsymbol{\eta}) \geq \mu(\|\mathbf{D}(\mathbf{x})\|^2) + 4\,\left(1-\frac{1}{n}\right)\mu'(\|\mathbf{D}(\mathbf{x})\|^2)\,\|\mathbf{D}(\mathbf{x})\|^2\,.$$

Due to $\mathbf{u} \in BUC^1(\mathbb{R}^n;\mathbb{R}^n)$ there is $M > 0$ such that $\|\mathbf{D}(\mathbf{x})\|^2 \leq M$ for all $\mathbf{x} \in \mathbb{R}^n$. Consequently, we obtain

$$\text{Re } (\mathcal{A}(\mathbf{x},\boldsymbol{\xi})\boldsymbol{\eta},\boldsymbol{\eta}) \geq \min_{s\in[0,M]}\left(\mu(s) + 4\left(1-\frac{1}{n}\right)\,s\,\mu'(s)\right) > 0$$

which proves the assertion. □

3.3.2 The Linear Problem with Constant Coefficients

Let $\mathcal{A}(D) = \sum_{k,l=1}^n A^{k,l}D_kD_l$ denote a differential operator of order 2 acting on $\mathbb{R}^n$-valued functions which will be identified with its L_p-realization whenever this is needed. Further, we assume that $\mathcal{A}(D)$ is strongly elliptic. Then, theorem 3.2.2 implies that for $J = [0,\tau] \subset \mathbb{R},\ \tau > 0$ the problem

$$\begin{array}{rcll} \frac{\partial}{\partial t}\mathbf{u} + \mathcal{A}(D)\mathbf{u} &=& \mathbf{f}(t,\mathbf{x}) & t \in J, \mathbf{x} \in \mathbb{R}^n, \\ \mathbf{u}(0,\mathbf{x}) &=& \mathbf{u}_0(\mathbf{x}) & \mathbf{x} \in \mathbb{R}^n \end{array} \tag{3.19}$$

has maximal L_p-regularity for any $1 < p < \infty$. In particular, for every $\mathbf{f} \in L_p(J\times\mathbb{R}^n;\mathbb{R}^n)$ and $\mathbf{u}_0 \in W_p^{2-2/p}(\mathbb{R}^n;\mathbb{R}^n)$ there is a unique solution $\mathbf{u}$ of system (3.19) in the class $\mathbf{u} \in H_p^1(J;L_p(\mathbb{R}^n;\mathbb{R}^n)) \cap L_p(J;H_p^2(\mathbb{R}^n;\mathbb{R}^n))$.

The next result shows that a similar statement holds for the generalized Stokes problem on $\mathbb{R}^n$, by which we mean the problem

$$\begin{array}{rcll} \frac{\partial}{\partial t}\mathbf{u} + \mathcal{A}(D)\mathbf{u} + \nabla p &=& \mathbf{f}(t,\mathbf{x}) & t \in J, \mathbf{x} \in \mathbb{R}^n \\ \operatorname{div}\mathbf{u} &=& g(t,\mathbf{x}) & t \in J, \mathbf{x} \in \mathbb{R}^n \\ \mathbf{u}(0,\mathbf{x}) &=& \mathbf{u}_0(\mathbf{x}) & \mathbf{x} \in \mathbb{R}^n. \end{array} \tag{3.20}$$

For the definition of the spaces $\dot{H}_p^1(\mathbb{R}^n)$ and $\dot{H}_p^{-1}(\mathbb{R}^n)$, we remind the reader of (3.3).

Theorem 3.3.2 *Let $n \in \mathbb{N},\ J = [0,\tau]$ with $\tau > 0$ and $1 < p < \infty$. Suppose that $\mathcal{A}(D) = \sum_{k,l=1}^n A^{k,l}D_kD_l$ is strongly elliptic with angle of ellipticity $\phi_{\mathcal{A}}$. Then, system (3.20) has maximal regularity in the following sense. There is a unique solution $(\mathbf{u},p)$ of system (3.20) within the class*

$$\mathbf{u} \in H_p^1(J;L_p(\mathbb{R}^n;\mathbb{R}^n)) \cap L_p(J;H_p^2(\mathbb{R}^n;\mathbb{R}^n)), \qquad p \in L_p(J;\dot{H}_p^1(\mathbb{R}^n))$$

if and only if the data $\mathbf{f}, g,$ and $\mathbf{u}_0$ satisfy the following conditions,

(i) $\mathbf{f} \in L_p(J\times\mathbb{R}^n;\mathbb{R}^n)$;

(ii) $g \in H_p^1(J;\dot{H}_p^{-1}(\mathbb{R}^n)) \cap L_p(J;H_p^1(\mathbb{R}^n))$;

(iii) $\mathbf{u}_0 \in W_p^{2-2/p}(\mathbb{R}^n;\mathbb{R}^n)$ *and* $\operatorname{div}\mathbf{u}_0 = g_{|t=0}$.

The solution $(\mathbf{u},p)$ *depends continuously on the data with respect to the corresponding norms.*

Proof. Concerning necessity: the conditions (i), (ii) on the data follow directly from the regularity of $(\mathbf{u},p)$. Condition (iii) follows from the trace theorem.

In order to prove sufficiency, it is enough to obtain solvability of system (3.20). Then, the continuity assertion follows from the open mapping theorem.

Let $\mathbf{f}$, g and $\mathbf{u}_0$ be given such that $(i)-(iii)$ are valid. Since $\mathcal{A}(D)$ is strongly elliptic, theorem 3.2.2 yields a solution $\mathbf{v}$ of problem (3.19) which has the property of maximal regularity. Then, $\mathbf{u} := \mathbf{v}+\mathbf{w}$ is a solution of system (3.20), provided that $\mathbf{w}$ is a solution of the problem

$$\begin{aligned} \tfrac{\partial}{\partial t}\mathbf{w} + \mathcal{A}(D)\mathbf{w} + \nabla p &= 0 && t\in J, \mathbf{x}\in\mathbb{R}^n \\ \operatorname{div}\mathbf{w} &= h && t\in J, \mathbf{x}\in\mathbb{R}^n \\ \mathbf{w}_{|t=0} &= 0 && \mathbf{x}\in\mathbb{R}^n, \end{aligned} \tag{3.21}$$

where $h := g - \operatorname{div}\mathbf{v}$ has the regularity

$$h \in {}_0H_p^1(J;\dot{H}_p^{-1}(\mathbb{R}^n)) \cap L_p(J;H_p^1(\mathbb{R}^n)) \tag{3.22}$$

due to (iii).

In order to achieve a unique solution for system (3.21), we develop at first a solution formula for $(\mathbf{w},p)$ via transform methods. Taking the Laplace transform of $\mathbf{w}(t,\mathbf{x})$ with respect to t, defined by $\tilde{\mathbf{w}}(\lambda,\mathbf{x})$, we obtain

$$\begin{aligned} (\lambda+\mathcal{A}(D))\,\tilde{\mathbf{w}} &= -\nabla\tilde{p} \\ \operatorname{div}\tilde{\mathbf{w}} &= \tilde{h}. \end{aligned}$$

Then, we apply the Fourier transform to $\tilde{\mathbf{w}}(\lambda,\mathbf{x})$ with respect to $\mathbf{x}$, defined by $\mathcal{F}\tilde{\mathbf{w}}(\lambda,\boldsymbol{\xi})$. For a better readability, we set $\widehat{\mathbf{w}} := \mathcal{F}\tilde{\mathbf{w}}(\lambda,\boldsymbol{\xi})$, $\widehat{p} := \mathcal{F}\tilde{p}(\lambda,\boldsymbol{\xi})$, and $\widehat{h} := \mathcal{F}\tilde{h}(\lambda,\boldsymbol{\xi})$ for the Fourier-Laplace transforms. Thus, we obtain

$$(\lambda+\mathcal{A}(\boldsymbol{\xi}))\,\widehat{\mathbf{w}} = -i\boldsymbol{\xi}\widehat{p} \tag{3.23-a}$$

$$\langle i\boldsymbol{\xi},\widehat{\mathbf{w}}\rangle = \widehat{h} \tag{3.23-b}$$

with $\boldsymbol{\xi}\in\mathbb{R}^n\backslash\{0\}$. Due to strong ellipticity of $\mathcal{A}(D)$, the inverse of $(\lambda+\mathcal{A}(\boldsymbol{\xi}))$ exists for all $\lambda\in\Sigma_{\pi-\phi}$ provided that $\phi_{\mathcal{A}} < \phi < \pi/2$. Below, ϕ will always denote such an angle. Thus, we get the representation

$$\widehat{\mathbf{w}} = -i\left(\lambda+\mathcal{A}(\boldsymbol{\xi})\right)^{-1}\boldsymbol{\xi}\,\widehat{p} \qquad \text{for } \lambda\in\Sigma_{\pi-\phi}. \tag{3.24}$$

Inserting $\widehat{\mathbf{w}}$ in the divergence equation (3.23-b) results in

$$\left\langle \boldsymbol{\xi}, \left(\lambda+\mathcal{A}(\boldsymbol{\xi})\right)^{-1}\boldsymbol{\xi}\right\rangle \widehat{p} = \widehat{h}. \tag{3.25}$$

In order to get a representation for $\widehat{p}$, we define

$$\alpha(\lambda,\boldsymbol{\xi}) := \Big(\big(\lambda+\mathcal{A}(\boldsymbol{\xi})\big)^{-1}\boldsymbol{\xi},\boldsymbol{\xi}\Big) \qquad \text{for} \quad \lambda\in\Sigma_{\pi-\phi},\ \boldsymbol{\xi}\in\mathbb{R}^n$$

and show when $\alpha(\lambda,\boldsymbol{\xi})\neq 0$ holds. For this purpose, let $\boldsymbol{\eta} := (\lambda+\mathcal{A}(\boldsymbol{\xi}))^{-1}\boldsymbol{\xi}$. Then, we obtain

$$\alpha(\lambda,\boldsymbol{\xi}) = (\boldsymbol{\eta},(\lambda+\mathcal{A}(\boldsymbol{\xi}))\boldsymbol{\eta}) = \overline{\lambda}\,|\boldsymbol{\eta}|^2 + (\boldsymbol{\eta},\mathcal{A}(\boldsymbol{\xi})\boldsymbol{\eta})\,.$$

Thus,

$$\text{Re}\ \alpha(\lambda,\boldsymbol{\xi}) = \text{Re}\ \lambda\,|\boldsymbol{\eta}|^2 + \text{Re}\ \ (\boldsymbol{\eta},\mathcal{A}(\boldsymbol{\xi})\boldsymbol{\eta}) > 0 \quad \text{for}\ \lambda\in\Sigma_{\pi-\phi},\ \boldsymbol{\xi}\in\mathbb{R}^n$$

provided that $\boldsymbol{\eta}\neq 0$ and for the right choice of $\phi_{\mathcal{A}}<\phi<\pi/2$. By definition of $\boldsymbol{\eta}$, the case $\boldsymbol{\eta}=0$ can only occur if $\boldsymbol{\xi}=0$. Therefore,

$$\alpha(\lambda,\boldsymbol{\xi})\neq 0 \quad \text{for all} \quad \lambda\in\Sigma_{\pi-\phi},\ \boldsymbol{\xi}\in\mathbb{R}^n\backslash\{0\}. \tag{3.26}$$

Assuming that (3.26) holds, we may solve (3.25) for $\widehat{p}$ and (3.24) for $\widehat{\mathbf{w}}$ such that we obtain

$$\widehat{p} = \frac{1}{\alpha(\lambda,\boldsymbol{\xi})}\widehat{h} \qquad \text{and} \qquad \widehat{\mathbf{w}} = -i\,\frac{\big(\lambda+\mathcal{A}(\boldsymbol{\xi})\big)^{-1}\boldsymbol{\xi}}{\alpha(\lambda,\boldsymbol{\xi})}\,\widehat{h}.$$

In order to get a representation of $(\mathbf{w},p)$ itself, we apply theorem 3.2.1 to obtain a solution

$$\mathbf{v}_0 \in\ {}_0H^1_p(J;L_p(\mathbb{R}^n;\mathbb{R}^n))\cap L_p(J;H^2_p(\mathbb{R}^n;\mathbb{R}^n))$$

of the problem

$$\text{div}\,\mathbf{v}_0 = h,$$

which is possible due to (3.22). Exploitation of $\widehat{h}=\langle i\boldsymbol{\xi},\widehat{\mathbf{v}}_0\rangle$ yields

$$\widehat{\mathbf{w}} = \frac{\big(\lambda+\mathcal{A}(\boldsymbol{\xi})\big)^{-1}\boldsymbol{\xi}\otimes\boldsymbol{\xi}}{\alpha(\lambda,\boldsymbol{\xi})}\,\widehat{\mathbf{v}}_0 \qquad \text{and} \qquad \widehat{p} = \left\langle\frac{i\,\boldsymbol{\xi}}{\alpha(\lambda,\boldsymbol{\xi})},\widehat{\mathbf{v}}_0\right\rangle.$$

In order to show that $(\mathbf{w},p)$ has the desired maximal regularity, we have to study $(\partial_t-\Delta)\mathbf{w}$ and ∇p. On the transformed side, this corresponds to

$$(\lambda+|\boldsymbol{\xi}|^2)\widehat{\mathbf{w}} = \frac{\big(\lambda+\mathcal{A}(\boldsymbol{\xi})\big)^{-1}\boldsymbol{\xi}\otimes\boldsymbol{\xi}}{\alpha(\lambda,\boldsymbol{\xi})}(\lambda+|\boldsymbol{\xi}|^2)\widehat{\mathbf{v}}_0, \tag{3.27-a}$$

$$i\,\boldsymbol{\xi}\,\widehat{p} = -\frac{\boldsymbol{\xi}\otimes\boldsymbol{\xi}}{\alpha(\lambda,\boldsymbol{\xi})}\,\widehat{\mathbf{v}}_0. \tag{3.27-b}$$

This yields the representation

$$(\partial_t-\Delta)\mathbf{w} = T_1(\partial_t-\Delta)\mathbf{v}_0 \tag{3.28-a}$$

$$\nabla p = T_2(\partial_t-\Delta)\mathbf{v}_0, \tag{3.28-b}$$

where T_1 and T_2 are multiplier operators that are defined by means of their Fourier-Laplace symbols $\mathcal{M}_1$ and $\mathcal{M}_2$, respectively. According to (3.27), the symbols are given by

$$\mathcal{M}_1(\lambda,\boldsymbol{\xi}) = \frac{\big(\lambda+\mathcal{A}(\boldsymbol{\xi})\big)^{-1}\boldsymbol{\xi}\otimes\boldsymbol{\xi}}{\alpha(\lambda,\boldsymbol{\xi})} \qquad \text{and} \qquad \mathcal{M}_2(\lambda,\boldsymbol{\xi}) = -\frac{\boldsymbol{\xi}\otimes\boldsymbol{\xi}}{(\lambda+|\boldsymbol{\xi}|^2)\alpha(\lambda,\boldsymbol{\xi})}$$

In order to finish the proof, it is sufficient to show that the operators T_1 and T_2 defined by (3.28) belong to $\mathcal{B}(L_p(J\times\mathbb{R}^n;\mathbb{R}^n))$. For this purpose, we first show that α^{-1} is bounded. We already know that $\alpha(\lambda,\boldsymbol{\xi})\neq 0$ for all $\boldsymbol{\xi}\in\mathbb{R}^n\backslash\{0\}$ with $|\boldsymbol{\xi}|=1$ and $\lambda\in\Sigma_{\pi-\phi}$ by (3.26). The $\mathcal{M}_i$ satisfy the following "parabolic homogeneity".

$$\mathcal{M}_i(\lambda,\boldsymbol{\xi}) = \mathcal{M}_i(\mu,\boldsymbol{\zeta}) \qquad \text{for } \boldsymbol{\zeta} := \boldsymbol{\xi}/|\boldsymbol{\xi}|\,,\ \mu := \lambda/|\boldsymbol{\xi}|^2\,,\ i=1,2.$$

For $|\mu|\leq R,\ R>0$ we get uniform boundedness of $\mathcal{M}_i$, since the denominator does not vanish. In case of $|\mu|\to\infty$ we extend symbol $\mathcal{M}_1$ with μ and take into consideration that $\mu\big(\mu+\mathcal{A}(\boldsymbol{\zeta})\big)^{-1}\to\mathbf{I}$ as $|\mu|\to\infty$, uniformly in $\boldsymbol{\zeta}\in S^{n-1}$. Thus, we obtain

$$\frac{\mu\big(\mu+\mathcal{A}(\boldsymbol{\zeta})\big)^{-1}}{\Big(\mu\big(\mu+\mathcal{A}(\boldsymbol{\zeta})\big)^{-1}\boldsymbol{\zeta},\boldsymbol{\zeta}\Big)}\to|\boldsymbol{\zeta}|^{-2}=1 \quad \text{as} \quad |\mu|\to\infty$$

for the μ dependent part of symbol $\mathcal{M}_1$ as well as

$$(1+\mu)\,\alpha(\mu,\boldsymbol{\zeta}) = (\mu^{-1}+1)\Big(\mu\big(\mu+\mathcal{A}(\boldsymbol{\zeta})\big)^{-1}\boldsymbol{\zeta},\boldsymbol{\zeta}\Big)\to|\boldsymbol{\zeta}|^2=1 \quad \text{as} \quad |\mu|\to\infty \tag{3.29}$$

for the μ dependent part of symbol $\mathcal{M}_2$. From these considerations we infer that

$$\sup\Big\{\,|\mathcal{M}_i(\lambda,\boldsymbol{\xi})|:\ \lambda\in\Sigma_{\pi-\phi},\ \boldsymbol{\xi}\in\mathbb{R}^n\backslash\{0\}\Big\}<\infty \quad \text{for} \quad i=1,2. \tag{3.30}$$

Furthermore, differentiation of the identity

$$\mathcal{M}_i(s^2\mu,s\boldsymbol{\zeta}) = \mathcal{M}_i(\mu,\boldsymbol{\zeta}) \qquad \text{for all } s>0$$

yields

$$s\,\partial_{\xi_k}\mathcal{M}_i(s^2\mu,s\boldsymbol{\zeta}) = \partial_{\xi_k}\mathcal{M}_i(\mu,\boldsymbol{\zeta})$$

and therefore

$$\partial_{\xi_k}\mathcal{M}_i(\lambda,\boldsymbol{\xi}) = |\boldsymbol{\xi}|^{-1}\,\partial_{\xi_k}\mathcal{M}_i(\mu,\boldsymbol{\zeta}).$$

This shows that

$$\Big|D^\beta_{\boldsymbol{\xi}}\mathcal{M}_i(\lambda,\boldsymbol{\xi})\Big| \leq |\boldsymbol{\xi}|^{-|\beta|}\ \sup\Big\{\Big|D^\beta_{\boldsymbol{\xi}}\mathcal{M}_i(\mu,\boldsymbol{\zeta})\Big|:\mu\in\Sigma_{\pi-\phi},\ |\boldsymbol{\zeta}|=1\Big\} \tag{3.31}$$

for every multi-index $\beta\in\mathbb{N}_0^n$ and $i=1,2$. The supremum on the right-hand side of (3.31) is finite by analogous considerations for $|\mu|\to\infty$ as above. Due to the estimate (3.31), the classical Mikhlin multiplier theorem 3.2.3 implies that the symbols $\mathcal{M}_i(\lambda,\cdot)$ are Fourier

multipliers in $L_p(\mathbb{R}^n;\mathbb{R}^n)$ with respect to the variable $\boldsymbol{\xi}$. This yields a uniformly bounded and holomorphic family

$$\{\mathcal{T}_i(\lambda)\}_{\lambda\in\Sigma_{\pi-\phi}} \subset \mathcal{B}(L_p(\mathbb{R}^n;\mathbb{R}^n))$$

for $\phi_{\mathcal{A}} < \phi < \pi/2$. Moreover, the estimates (3.30) and (3.31) lead to a bounded set $\tau \subset \mathbb{R}^{n\times n} = \mathcal{B}(\mathbb{R}^n)$ such that for all $\beta \in \mathbb{N}_0^n$ with $|\beta| \le [n/q]+1$ and $q \in [1,2]$ the inclusion

$$|\boldsymbol{\xi}|^{|\beta|} D_{\boldsymbol{\xi}}^{\beta}\mathcal{M}_i(\lambda,\boldsymbol{\xi}) \in \tau \quad \text{ for all } \boldsymbol{\xi}\in\mathbb{R}^n\backslash\{0\},\ \lambda\in\Sigma_{\pi-\phi}$$

is valid. Since a bounded set in $\mathcal{B}(\mathbb{R}^n)$ is also $\mathcal{R}$-bounded, we have

$$\mathcal{R}(\tau) < \infty$$

and therefore theorem 3.2.4 is applicable and yields

$$\mathcal{R}\left(\{\mathcal{T}_i(\lambda)\}_{\lambda\in\Sigma_{\pi-\phi}}\right) < \infty \quad \text{for } i=1,2.$$

The operators $\mathcal{T}_i(\lambda)$ extend to operators on $L_p(J\times\mathbb{R}^n;\mathbb{R}^n)$, again denoted by $\mathcal{T}_i(\lambda)$, simply by means of

$$\left(\mathcal{T}_i(\lambda)\mathbf{f}\right)(t,\mathbf{x}) = \left(\mathcal{T}_i(\lambda)\mathbf{f}(t,\cdot)\right)(\mathbf{x})$$

and then $\{\mathcal{T}_i(\lambda)\}_{\lambda\in\Sigma_{\pi-\phi}}$ is again $\mathcal{R}$-bounded in $\mathcal{B}(L_p(J\times\mathbb{R}^n;\mathbb{R}^n))$ by proposition 3.2.3. The operators $\mathcal{T}_i(\lambda)$ are related to the operators T_i by means of $T_i = \mathcal{T}_i(\partial_t)$. In order to show that ∂_t can be inserted into the holomorphic vector-valued function $\mathcal{T}_i(\lambda)$, we are going to apply theorem 3.2.5. By proposition 3.2.4 the operator ∂_t in $L_p(J;X)$ with $X = L_p(\mathbb{R}^n;\mathbb{R}^n)$ and natural domain ${}_0H_p^1(J;X)$ admits a bounded $\mathcal{H}^\infty$-calculus with $\mathcal{H}^\infty$-angle $\pi/2$. The resolvents of ∂_t commute with $\mathcal{T}_i(\lambda)$, since the latter operators correspond to the space variable. Finally, due to $\pi-\phi > \pi/2$ theorem 3.2.5 is applicable. Hence, $T_i = \mathcal{T}_i(\partial_t)$ are bounded in $L_p(J;X)$. □

This theorem can be extended to the case of variable coefficients which arise from constant ones by small perturbations, i.e., for

$$\mathcal{A}(t,\mathbf{x},D) = \mathcal{A}_0(D) + \mathcal{A}_1(t,\mathbf{x},D),$$

where $\mathcal{A}_0$ is as in theorem 3.3.2 and

$$\mathcal{A}_1(t,\mathbf{x},D) = \sum_{k,l=1}^{n} A_1^{k,l}(t,\mathbf{x})\ D_kD_l \qquad \text{with } A_1^{k,l}(t,\mathbf{x}) = \left(a_{1,i,j}^{k,l}(t,\mathbf{x})\right) \tag{3.32}$$

and

$$\sup\left\{\left|a_{1,i,j}^{k,l}(t,\mathbf{x})\right| :\ i,j,k,l=1,\dots,n,\ t\in J,\ \mathbf{x}\in\mathbb{R}^n\right\} \le \eta. \tag{3.33}$$

Indeed, we have the following result.

Corollary 3.3.1 *Let $n \in \mathbb{N}, J = [0,\tau]$ with $\tau > 0$ and $1 < p < \infty$. Suppose that*

$$\mathcal{A}(t,\mathbf{x},D) = \mathcal{A}_0(D) + \mathcal{A}_1(t,\mathbf{x},D)$$

with $\mathcal{A}_0$ as in theorem 3.3.2 and $\mathcal{A}_1$ of type (3.32) with measurable coefficients. Then, there is $\eta_0 > 0$ such that the assertions of theorem 3.3.2 remain valid, provided that (3.33) holds with $\eta < \eta_0$.

Proof. In order to obtain a better readability, we introduce the following abbreviations

$$\begin{aligned} X :=& L_p(J\times\mathbb{R}^n;\mathbb{R}^n),\\ Y :=& H_p^1(J;\dot{H}_p^{-1}(\mathbb{R}^n)) \cap L_p(J;H_p^1(\mathbb{R}^n)),\\ X_p :=& W_p^{2-2/p}(\mathbb{R}^n;\mathbb{R}^n). \end{aligned}$$

Furthermore, let

$$Z := \Big(H_p^1(J;L_p(\mathbb{R}^n;\mathbb{R}^n)) \cap L_p(J;H_p^2(\mathbb{R}^n;\mathbb{R}^n))\Big) \times L_p(J;\dot{H}_p^1(\mathbb{R}^n)),$$

and $S : X \times Y \times X_p \to Z$ denote the solution operator of the generalized Stokes problem (3.20) with $\mathcal{A}_0(D)$ instead of $\mathcal{A}(D)$. If the perturbed problem is solvable with solution operator T, then

$$T = S - SBT \qquad \text{with} \quad B = \begin{bmatrix} \mathcal{A}_1(t,\mathbf{x},D) & 0\\ 0 & 0\\ 0 & 0 \end{bmatrix}. \tag{3.34}$$

Here, $B : Z \to X \times Y \times X_p$ is bounded by $C\eta > 0$, where $C > 0$ is a constant which does not depend on η. Let $\eta_0 = (|S|\,C)^{-1}$, where $|S|$ denotes the operator norm of S. Then, $\eta < \eta_0$ implies $|SB|_{\mathcal{B}(Z)} < 1$, hence $\mathbf{I} + SB$ has an inverse $(\mathbf{I}+SB)^{-1} \in \mathcal{B}(Z)$ which is given as a Neumann series. Hence, $T = (\mathbf{I}+SB)^{-1}S$ solves the operator equation (3.34).

In order to see that T is indeed the solution operator of the perturbed problem, let

$$\begin{bmatrix}\mathbf{u}\\ p\end{bmatrix} = T\begin{bmatrix}\mathbf{f}\\ g\\ \mathbf{u}_0\end{bmatrix} \qquad \text{for} \quad \mathbf{f}\in X, g\in Y, \text{ and } \mathbf{u}_0 \in X_p.$$

Then, $(\mathbf{u},p) \in Z$ and

$$\begin{bmatrix}\mathbf{u}\\ p\end{bmatrix} + SB\begin{bmatrix}\mathbf{u}\\ p\end{bmatrix} = S\begin{bmatrix}\mathbf{f}\\ g\\ \mathbf{u}_0\end{bmatrix}.$$

By definition of the operator B, $(\mathbf{u},p)$ solves

$$\begin{aligned} \partial_t\mathbf{u} + \mathcal{A}_0(D)\mathbf{u} + \nabla p + \mathcal{A}_1(t,\mathbf{x},D)\mathbf{u} &= \mathbf{f}\\ \operatorname{div}\mathbf{u} &= g\\ \mathbf{u}_{|_{t=0}} &= \mathbf{u}_0. \end{aligned}$$

□

3.3.3 The Linear Problem with Variable Coefficients

We consider the fully inhomogeneous initial boundary value problem

$$\begin{aligned} \tfrac{\partial}{\partial t}\mathbf{u} + \mathcal{A}(t,\mathbf{x},D)\mathbf{u} + \nabla p &= \mathbf{f}(t,\mathbf{x}) && t \in J, \mathbf{x} \in \mathbb{R}^n \\ \operatorname{div}\mathbf{u} &= g && t \in J, \mathbf{x} \in \mathbb{R}^n \\ \mathbf{u}(0,\mathbf{x}) &= \mathbf{u}_0(\mathbf{x}) && \mathbf{x} \in \mathbb{R}^n, \end{aligned} \tag{3.35}$$

where $J = [0,\tau]$ with $\tau > 0$ and

$$\mathcal{A}(t,\mathbf{x},D) = \sum_{k,l=1}^{n} A^{k,l}(t,\mathbf{x}) D_k D_l$$

denotes a strongly elliptic differential operator. We suppose that the coefficients $A^{k,l}(t,\mathbf{x})$ are continuous on $J \times \mathbb{R}^n$ with limits $A^{k,l}(t,\infty)$ for $|\mathbf{x}| \to \infty$, uniformly in $t \in J$, such that $A(t,\infty,D)$ is strongly elliptic as well. Then, theorem 3.3.2 can be extended to this variable case, i.e., problem (3.35) has a unique solution $(\mathbf{u},p)$ within the class

$$\mathbf{u} \in H^1_p(J; L_p(\mathbb{R}^n;\mathbb{R}^n)) \cap L_p(J; H^2_p(\mathbb{R}^n;\mathbb{R}^n)), \quad p \in L_p(J; \dot{H}^1_p(\mathbb{R}^n)),$$

if and only if the data $\mathbf{f}, g$, and $\mathbf{u}_0$ satisfy

(i) $\mathbf{f} \in L_p(J \times \mathbb{R}^n;\mathbb{R}^n)$,

(ii) $g \in H^1_p(J; \dot{H}^{-1}_p(\mathbb{R}^n)) \cap L_p(J; H^1_p(\mathbb{R}^n))$,

(iii) $\mathbf{u}_0 \in W^{2-2/p}_p(\mathbb{R}^n;\mathbb{R}^n)$ and $\operatorname{div}\mathbf{u}_0 = g_{|t=0}$.

The proof will be based on localization methods and corollary 3.3.1. The latter will be applied to a right-hand side which, for example, contains a term $p\nabla\varphi_k$ within the evolution equation for the velocity, where φ_k stems from a partition of unity. Such a term is problematic, since it is neither of lower order nor a small highest order term. The point here is, that the pressure p has no better time regularity than L_p. On the other hand, the spatial regularity is one order higher than L_p and a part of the solution operator shifts this into additional time regularity. Therefore, the strategy is to exploit the fact that the solution operator S of the generalized Stokes problem

$$\begin{aligned} \tfrac{\partial}{\partial t}\mathbf{u} + \mathcal{A}(D)\mathbf{u} + \nabla p &= \mathbf{f}(t,\mathbf{x}) && t \in J, \mathbf{x} \in \mathbb{R}^n \\ \operatorname{div}\mathbf{u} &= g(t,\mathbf{x}) && t \in J, \mathbf{x} \in \mathbb{R}^n \\ \mathbf{u}(0,\mathbf{x}) &= \mathbf{u}_0(\mathbf{x}) && \mathbf{x} \in \mathbb{R}^n, \end{aligned}$$

splits as $S = S_0 + S_1$, where S_0 is independent of the coefficients of $\mathcal{A}(D)$ and S_1 shuffles between temporal and spatial regularity.

In order to obtain the Fourier-Laplace symbols of S_0 and S_1 , observe that analogously to the proof of theorem 3.3.2 we get the representation

$$\begin{bmatrix} \widehat{\mathbf{u}} \\ \widehat{p} \end{bmatrix} = \mathcal{S}(\lambda,\boldsymbol{\xi}) \begin{bmatrix} \widehat{\mathbf{f}} \\ \widehat{g} \end{bmatrix} \tag{3.36}$$

with

$$\mathcal{S}(\lambda,\boldsymbol{\xi}) = \begin{bmatrix} \left(\mathbf{I} - \dfrac{\left(\lambda+\mathcal{A}(\boldsymbol{\xi})\right)^{-1}\boldsymbol{\xi}\otimes\boldsymbol{\xi}}{\alpha(\lambda,\boldsymbol{\xi})}\right)\left(\lambda+\mathcal{A}(\boldsymbol{\xi})\right)^{-1} & \dfrac{-i\left(\lambda+\mathcal{A}(\boldsymbol{\xi})\right)^{-1}\boldsymbol{\xi}}{\alpha(\lambda,\boldsymbol{\xi})} \\ -i\dfrac{1}{\alpha(\lambda,\boldsymbol{\xi})}\left(\left(\lambda+\mathcal{A}(\boldsymbol{\xi})\right)^{-1}\bullet,\boldsymbol{\xi}\right) & \dfrac{1}{\alpha(\lambda,\boldsymbol{\xi})} \end{bmatrix}$$

in case of $\mathbf{u}_0 = 0$.

To obtain the decomposition of $\mathcal{S}$, we first study the term $1/\alpha(\lambda,\boldsymbol{\xi})$, using again the notation $\mu = \lambda/|\boldsymbol{\xi}|^2$ and $\boldsymbol{\zeta} = \boldsymbol{\xi}/|\boldsymbol{\xi}|$. Due to (3.29),we consider

$$\begin{aligned}\frac{1}{\alpha(\lambda,\boldsymbol{\xi})} - (1+\mu) =& \frac{1}{\alpha(\lambda,\boldsymbol{\xi})}\left(1-(1+\mu)\alpha(\lambda,\boldsymbol{\xi})\right)\\ =& \frac{1}{\alpha(\lambda,\boldsymbol{\xi})}\left((\boldsymbol{\zeta},\boldsymbol{\zeta}) - (1+\mu)\left(\left(\mu+\mathcal{A}(\boldsymbol{\zeta})\right)^{-1}\boldsymbol{\zeta},\boldsymbol{\zeta}\right)\right)\\ =& \frac{1}{\alpha(\lambda,\boldsymbol{\xi})}\left(\left(\mathbf{I}-(1+\mu)\left(\mu+\mathcal{A}(\boldsymbol{\zeta})\right)^{-1}\right)\boldsymbol{\zeta},\boldsymbol{\zeta}\right)\\ =& \frac{1}{\alpha(\lambda,\boldsymbol{\xi})}\left(\left(\mathcal{A}(\boldsymbol{\zeta})-1\right)\left(\mu+\mathcal{A}(\boldsymbol{\zeta})\right)^{-1}\boldsymbol{\zeta},\boldsymbol{\zeta}\right),\end{aligned}$$

hence

$$\frac{1}{\alpha(\lambda,\boldsymbol{\xi})} = \frac{\lambda}{|\boldsymbol{\xi}|^2} + 1 + \mathcal{M}_{22}(\lambda,\boldsymbol{\xi}) \tag{3.37}$$

with

$$\mathcal{M}_{22}(\lambda,\boldsymbol{\xi}) = \frac{1}{\alpha(\lambda,\boldsymbol{\xi})}\left(\left(\mathcal{A}(\boldsymbol{\xi}/|\boldsymbol{\xi}|)-1\right)\left(\lambda+\mathcal{A}(\boldsymbol{\xi})\right)^{-1}\boldsymbol{\xi},\boldsymbol{\xi}\right).$$

As in the proof of theorem 3.3.2, the symbol $\mathcal{M}_{22}$ satisfies

$$\mathcal{M}_{22}(s^2\lambda, s\boldsymbol{\xi}) = \mathcal{M}_{22}(\lambda,\boldsymbol{\xi}) \quad \text{for} \quad \boldsymbol{\xi}\in\mathbb{R}^n\backslash\{0\},\ \lambda\in\Sigma_{\pi-\phi},\ s>0.$$

Moreover, $\mathcal{M}_{22}$ is bounded, uniformly in $\boldsymbol{\xi}\in\mathbb{R}^n\backslash\{0\}$ and $\lambda\in\Sigma_{\pi-\phi}$. Then, a repetition of the arguments given there shows that $\mathcal{M}_{22}$ is the Fourier-Laplace symbol of an operator $S_{22}\in\mathcal{B}(L_p(J\times\mathbb{R}^n))$. In a similar way, we obtain

$$-i\frac{1}{\alpha(\lambda,\boldsymbol{\xi})}\left(\lambda+\mathcal{A}(\boldsymbol{\xi})\right)^{-1}\boldsymbol{\xi} = -i\frac{\boldsymbol{\xi}}{|\boldsymbol{\xi}|^2} + \frac{|\boldsymbol{\xi}|}{\lambda+|\boldsymbol{\xi}|^2}\mathcal{M}_{12}(\lambda,\boldsymbol{\xi}), \tag{3.38}$$

where

$$\mathcal{M}_{12}(\lambda,\boldsymbol{\xi}) = i\left(\frac{\mathcal{A}(\boldsymbol{\xi})}{|\boldsymbol{\xi}|^2} - \mathcal{M}_{22}(\lambda,\boldsymbol{\xi}) - 1\right)\left(\lambda+\mathcal{A}(\boldsymbol{\xi})\right)^{-1}(\lambda+|\boldsymbol{\xi}|^2)\frac{\boldsymbol{\xi}}{|\boldsymbol{\xi}|}$$

is the symbol of an operator $S_{12}\in\mathcal{B}(L_p(J\times\mathbb{R}^n;\mathbb{R}^n))$. For the next entry we use

$$-i\frac{1}{\alpha(\lambda,\boldsymbol{\xi})}\left(\left(\lambda+\mathcal{A}(\boldsymbol{\xi})\right)^{-1}\bullet,\boldsymbol{\xi}\right) = -i\frac{\boldsymbol{\xi}^T}{|\boldsymbol{\xi}|^2} + \frac{|\boldsymbol{\xi}|}{\lambda+|\boldsymbol{\xi}|^2}\mathcal{M}_{21}(\lambda,\boldsymbol{\xi}) \tag{3.39}$$

with

$$\mathcal{M}_{21}(\lambda,\boldsymbol{\xi}) = i\frac{\boldsymbol{\xi}^T}{|\boldsymbol{\xi}|}\left(\frac{\mathcal{A}(\boldsymbol{\xi})}{|\boldsymbol{\xi}|^2} - \mathcal{M}_{22}(\lambda,\boldsymbol{\xi}) - 1\right)\left(\lambda + \mathcal{A}(\boldsymbol{\xi})\right)^{-1}\left(\lambda + |\boldsymbol{\xi}|^2\right)$$

and $\mathcal{M}_{21}$ is the symbol of an operator $S_{21} \in \mathcal{B}(L_p(J\times\mathbb{R}^n;\mathbb{R}^n))$. Finally, using the relation (3.37) we obtain the decomposition

$$\left(\mathbf{I} - \frac{\left(\lambda + \mathcal{A}(\boldsymbol{\xi})\right)^{-1}\boldsymbol{\xi}\otimes\boldsymbol{\xi}}{\alpha(\lambda,\boldsymbol{\xi})}\right)\left(\lambda + \mathcal{A}(\boldsymbol{\xi})\right)^{-1}$$
$$= \frac{\mathbf{I} - \boldsymbol{\xi}/|\boldsymbol{\xi}|\otimes\boldsymbol{\xi}/|\boldsymbol{\xi}|}{\lambda + |\boldsymbol{\xi}|^2} + \frac{|\boldsymbol{\xi}|^2}{(\lambda+|\boldsymbol{\xi}|^2)^2}\mathcal{M}_{11}(\lambda,\boldsymbol{\xi}) \qquad (3.40)$$

with

$$\mathcal{M}_{11}(\lambda,\boldsymbol{\xi}) = \left\{\left(\mathbf{I} - \frac{\boldsymbol{\xi}\otimes\boldsymbol{\xi}}{|\boldsymbol{\xi}|^2}\right)\left(\mathbf{I} - \frac{\mathcal{A}(\boldsymbol{\xi})}{|\boldsymbol{\xi}|^2}\right) + \left(\frac{\mathcal{A}(\boldsymbol{\xi})}{|\boldsymbol{\xi}|^2} - \mathcal{M}_{22}(\lambda,\boldsymbol{\xi}) - 1\right)\right.$$
$$\left.\left[\mathbf{I} + \left(|\boldsymbol{\xi}|^2 - \mathcal{A}(\boldsymbol{\xi})\right)\left(\lambda + \mathcal{A}(\boldsymbol{\xi})\right)^{-1}\right]\frac{\boldsymbol{\xi}\otimes\boldsymbol{\xi}}{|\boldsymbol{\xi}|^2}\right\}\left[\mathbf{I} + \left(|\boldsymbol{\xi}|^2 - \mathcal{A}(\boldsymbol{\xi})\right)\left(\lambda + \mathcal{A}(\boldsymbol{\xi})\right)^{-1}\right].$$

and once more $\mathcal{M}_{11}$ is the symbol of an L_p-bounded operator S_{11}.

Inserting the decompositions (3.37)-(3.40) into the representation (3.36) yields

$$\mathcal{S}_0 = \begin{bmatrix} \frac{\mathbf{I}-\boldsymbol{\zeta}\otimes\boldsymbol{\zeta}}{\lambda+|\boldsymbol{\xi}|^2} & \frac{-i\boldsymbol{\xi}}{|\boldsymbol{\xi}|^2} \\ \frac{-i\boldsymbol{\xi}^T}{|\boldsymbol{\xi}|^2} & \frac{\lambda+|\boldsymbol{\xi}|^2}{|\boldsymbol{\xi}|^2} \end{bmatrix} \text{ and } \mathcal{S}_1 = \begin{bmatrix} \frac{|\boldsymbol{\xi}|^2}{(\lambda+|\boldsymbol{\xi}|^2)^2}\mathcal{M}_{11}(\lambda,\boldsymbol{\xi}) & \frac{|\boldsymbol{\xi}|}{\lambda+|\boldsymbol{\xi}|^2}\mathcal{M}_{12}(\lambda,\boldsymbol{\xi}) \\ \frac{|\boldsymbol{\xi}|}{\lambda+|\boldsymbol{\xi}|^2}\mathcal{M}_{21}(\lambda,\boldsymbol{\xi}) & \mathcal{M}_{22}(\lambda,\boldsymbol{\xi}) \end{bmatrix}$$

for the Fourier-Laplace symbols of S_0 and S_1. In the forthcoming proof, it is not only important that $\mathcal{S}_0$ is independent of the coefficients of $\mathcal{A}(D)$, but also that $\mathcal{S}_1$ can be factorized as

$$\mathcal{S}_1 = \begin{bmatrix} \frac{1}{\lambda+|\boldsymbol{\xi}|^2} & 0 \\ 0 & \frac{1}{|\boldsymbol{\xi}|} \end{bmatrix}\begin{bmatrix} \mathcal{M}_{11}(\lambda,\boldsymbol{\xi}) & \mathcal{M}_{12}(\lambda,\boldsymbol{\xi}) \\ \mathcal{M}_{21}(\lambda,\boldsymbol{\xi}) & \mathcal{M}_{22}(\lambda,\boldsymbol{\xi}) \end{bmatrix}\begin{bmatrix} \frac{|\boldsymbol{\xi}|^2}{\lambda+|\boldsymbol{\xi}|^2} & 0 \\ 0 & |\boldsymbol{\xi}| \end{bmatrix}.$$

Remarkably, the same type of decomposition of the solution operator is valid in the variable coefficient case $\mathcal{A}(t,\mathbf{x},D) = \mathcal{A}(D) + \mathcal{A}_1(t,\mathbf{x},D)$ considered in corollary 3.3.1. In order to see this, we recall that the solution operator T corresponding to this case is given by the Neumann series

$$T = \sum_{n=0}^{\infty}(-1)^n(SB)^nS = S_0 + S_1 + \sum_{n=1}^{\infty}(-1)^n(SB)^nS,$$

where B is given by $B = \begin{bmatrix} A_1 & 0 \\ 0 & 0 \end{bmatrix}$. By induction, we immediately obtain

$$(SB)^n = \begin{bmatrix} (S_{11}A_1)^n & 0 \\ S_{21}A_1(S_{11}A_1)^{n-1} & 0 \end{bmatrix}$$

and

$$(SB)^n S = \begin{bmatrix} (S_{11}A_1)^n S_{11} & (S_{11}A_1)^n S_{12} \\ S_{21}A_1(S_{11}A_1)^{n-1}S_{11} & S_{21}A_1(S_{11}A_1)^{n-1}S_{12} \end{bmatrix}. \tag{3.41}$$

Using the factorization of S given above, the entries on the right-hand side of (3.41) are of the following type.

$$\begin{aligned} (S_{11}A_1)^n S_{11} &= S_{11}(A_1S_{11})^{n-1}A_1(-\Delta)^{-1}R_{11}, \\ (S_{11}A_1)^n S_{12} &= S_{11}(A_1S_{11})^{n-1}A_1(-\Delta)^{-1}R_{12}, \\ S_{21}A_1(S_{11}A_1)^{n-1}S_{11} &= (-\Delta)^{-1/2}R_{21}(A_1S_{11})^{n-1}A_1(-\Delta)^{-1}R_{11}, \\ S_{21}A_1(S_{11}A_1)^{n-1}S_{12} &= (-\Delta)^{-1/2}R_{21}(A_1S_{11})^{n-1}A_1(-\Delta)^{-1}R_{12}, \end{aligned}$$

where the operators R_{11}, R_{12} and R_{21} are given by their Fourier-Laplace symbols according to

$$\begin{aligned} \mathcal{R}_{11}(\lambda,\boldsymbol{\xi}) &= \left(\mathbf{I} + \frac{\boldsymbol{\xi}\otimes\boldsymbol{\xi}}{|\boldsymbol{\xi}|^2} + \frac{|\boldsymbol{\xi}|^2}{\lambda+|\boldsymbol{\xi}|^2}\mathcal{M}_{11}(\lambda,\boldsymbol{\xi})\right)\frac{|\boldsymbol{\xi}|^2}{\lambda+|\boldsymbol{\xi}|^2}, \\ \mathcal{R}_{12}(\lambda,\boldsymbol{\xi}) &= \left(i\,\frac{\boldsymbol{\xi}}{|\boldsymbol{\xi}|} + \frac{|\boldsymbol{\xi}|^2}{\lambda+|\boldsymbol{\xi}|^2}\mathcal{M}_{12}(\lambda,\boldsymbol{\xi})\right)|\boldsymbol{\xi}|\,, \\ \mathcal{R}_{21}(\lambda,\boldsymbol{\xi}) &= \left(-i\,\frac{\boldsymbol{\xi}^T}{|\boldsymbol{\xi}|} + \frac{|\boldsymbol{\xi}|^2}{\lambda+|\boldsymbol{\xi}|^2}\mathcal{M}_{21}(\lambda,\boldsymbol{\xi})\right). \end{aligned}$$

Together with the Fourier-Laplace symbol

$$\mathcal{S}_{11} = \frac{1}{\lambda+|\boldsymbol{\xi}|^2}\left(\mathbf{I} + \frac{\boldsymbol{\xi}\otimes\boldsymbol{\xi}}{|\boldsymbol{\xi}|^2} + \frac{|\boldsymbol{\xi}|^2}{\lambda+|\boldsymbol{\xi}|^2}\mathcal{M}_{11}(\lambda,\boldsymbol{\xi})\right),$$

it follows that

$$T = S_0 + \begin{bmatrix} (\partial_t-\Delta)^{-1} & 0 \\ 0 & (-\Delta)^{-1/2} \end{bmatrix} \widetilde{S_1} \begin{bmatrix} (-\Delta)(\partial_t-\Delta)^{-1} & 0 \\ 0 & (-\Delta)^{1/2} \end{bmatrix} \tag{3.42}$$

with $\widetilde{S_1} \in \mathcal{B}(L_p(J\times\mathbb{R}^n;\mathbb{R}^{n+1}))$.

Exploiting these requirements, we are now able to prove the following result.

Theorem 3.3.3 *Let $n \in \mathbb{N}, J = [0,\tau]$ with $\tau > 0$ and $1 < p < \infty$. Suppose that $\mathcal{A}(t,\mathbf{x},D) = \sum_{k,l=1}^n A^{k,l}(t,\mathbf{x})D_kD_l$ is strongly elliptic with coefficients $A^{k,l} \in BUC(J\times\mathbb{R}^n)$ such that $A^{k,l}(t,\infty) := \lim_{|\mathbf{x}|\to\infty} A^{k,l}(t,\mathbf{x})$ exists, uniformly in $t \in J$, and $\mathcal{A}(t,\infty,D)$*

is strongly elliptic as well. Then, system (3.35) has maximal L_p-regularity, i.e., there is a unique solution $(\mathbf{u}, p)$ of (3.35) in the class

$$\mathbf{u} \in H^1_p(J; L_p(\mathbb{R}^n; \mathbb{R}^n)) \cap L_p(J; H^2_p(\mathbb{R}^n; \mathbb{R}^n)), \quad p \in L_p(J; \dot{H}^1_p(\mathbb{R}^n))$$

if and only if the data $\mathbf{f}, g$, and $\mathbf{u}_0$ satisfy

(i) $\mathbf{f} \in L_p(J \times \mathbb{R}^n; \mathbb{R}^n)$;

(ii) $g \in {}_0H^1_p(J; \dot{H}^{-1}_p(\mathbb{R}^n)) \cap L_p(J; H^1_p(\mathbb{R}^n))$;

(iii) $\mathbf{u}_0 \in W^{2-2/p}_p(\mathbb{R}^n; \mathbb{R}^n)$ *and* $\operatorname{div} \mathbf{u}_0 = g_{|t=0}$.

Proof. According to theorem 3.3.2, the generalized Stokes problem with coefficients frozen at any $t_0 \in J, \mathbf{x}_0 \in \mathbb{R}^n \cup \{\infty\}$ have maximal L_p-regularity, i.e., there is a constant $C > 0$ which is independent of the data $\mathbf{f}, g$, and $\mathbf{u}_0$ such that

$$|(\mathbf{u}, p)|_{Z_\tau} \le C \left(|\mathbf{f}|_{X_\tau} + |g|_{Y_\tau} + |\mathbf{u}_0|_{X_p} \right), \tag{3.43}$$

where

$$\begin{aligned}
X_\tau =& L_p(J \times \mathbb{R}^n; \mathbb{R}^n),\\
Y_\tau =& H^1_p(J; \dot{H}^{-1}_p(\mathbb{R}^n)) \cap L_p(J; H^1_p(\mathbb{R}^n)),\\
Z_\tau =& \Big(H^1_p(J; L_p(\mathbb{R}^n; \mathbb{R}^n)) \cap L_p(J; H^2_p(\mathbb{R}^n; \mathbb{R}^n)) \Big) \times L_p(J; \dot{H}^1_p(\mathbb{R}^n)),\\
X_p =& W^{2-2/p}_p(\mathbb{R}^n; \mathbb{R}^n).
\end{aligned}$$

Moreover, the maximal regularity constant C in inequality (3.43) can be chosen independently of $(t_0, \mathbf{x}_0) \in J \times (\mathbb{R}^n \cup \{\infty\})$ due to the uniform continuity of the coefficients of $A(t, \mathbf{x}, D)$. Hence, the norm of the corresponding solution operator is also uniformly bounded.

In order to achieve a solution of system (3.35), we first reduce the system to the case $\mathbf{f} = 0$ and $\mathbf{u}_0 = 0$ by theorem 3.2.2 as done in the proof of theorem 3.3.2. In order to show global existence in time, we divide the time interval $J = [0, \tau]$ in m time steps with $0 = \tau_0 < \tau_1 < \ldots < \tau_{m-1} < \tau_m = \tau$. W.l.o.g. we may assume that J is subdivided equidistantly, i.e., let $h = \tau/m$. Then, we solve problem (3.35) successively on each of the intervals $J_i = [\tau_i, \tau_{i+1}]$ for $i = 1, \ldots, m-1$ by means of localization with respect to the spacial variable. Then, it is sufficient to determine the solution on the first interval $J_0 = [0, \tau_1]$ and to show that, given the solution on $[0, \tau_i]$, the interval of existence can be prolonged by J_i.

Given $\eta \in (0, \eta_0/2)$ with η_0 from corollary 3.3.1 and $h = \tau/m$ for a sufficiently large $m \in \mathbb{N}$ such that all coefficients $a(t, \mathbf{x})$ appearing in $\mathcal{A}(t, \mathbf{x}, D)$ satisfy

$$\sup\Big\{ |a(s, \mathbf{x}) - a(t, \mathbf{x})| : \ \mathbf{x} \in \mathbb{R}^n, \ s, t \in J, \ |s - t| \le h \Big\} \le \eta.$$

In order to obtain the solution on J_0, we can choose a large $R > 0$ such that all coefficients $a(t, \mathbf{x})$ satisfy

$$\sup\Big\{|a(0,\mathbf{x}) - a(0,\infty)| : \ |\mathbf{x}| \geq R\Big\} \leq \eta,$$

and cover the ball $\overline{B_R(0)}$ by finitely many balls $B_r(\mathbf{x}_k),\ k = 1, \ldots, N$ such that

$$\sup\Big\{|a(0,\mathbf{x}) - a(0,\mathbf{x}_k)| : \ \mathbf{x} \in B_r(\mathbf{x}_k)\Big\} \leq \eta,$$

Choose a C^∞-partition of unity $\{\varphi_k\}_{k=0,\ldots,N}$ which is subordinate to the covering

$$\overline{B_R(0)}^c \cup \bigcup_{k=1}^{N} B_r(\mathbf{x}_k)$$

of $\mathbb{R}^n$; here the index $k = 0$ corresponds to the chart at infinity, i.e., to $\overline{B_R(0)}^c := \mathbb{R}^n \backslash \overline{B_R(0)}$.

Define local operators

$$\mathcal{A}_k(t, \mathbf{x}, D) := \mathcal{A}(t, R_k\mathbf{x}, D),$$

where the reflections R_k are given by

$$R_k\mathbf{x} = \begin{cases} \mathbf{x} & \text{if } \mathbf{x} \in \overline{B_r(\mathbf{x}_k)} \\ \mathbf{x}_k + r^2 \frac{\mathbf{x}-\mathbf{x}_k}{|\mathbf{x}-\mathbf{x}_k|^2} & \text{if } \mathbf{x} \notin \overline{B_r(\mathbf{x}_k)} \end{cases}$$

for $k = 1, \ldots, N$ and

$$R_0\mathbf{x} = \begin{cases} \mathbf{x} & \text{if } \mathbf{x} \notin \overline{B_R(0)} \\ R^2 \frac{\mathbf{x}}{|\mathbf{x}|^2} & \text{if } \mathbf{x} \in \overline{B_R(0)}. \end{cases}$$

Then, we freeze the coefficients of the local operator $\mathcal{A}_k(t, \mathbf{x}, D)$ at the point $(0, \mathbf{x}_k)$ and get the differential operators with constant coefficients

$$\mathcal{A}_{0,k}(D) := \mathcal{A}_k(0, \mathbf{x}_k, D)$$

for $k = 1, \ldots, N$ and

$$\mathcal{A}_{0,0}(D) := \mathcal{A}_0(0, \infty, D).$$

Then

$$\mathcal{A}_k(t, \mathbf{x}, D) = \mathcal{A}_{0,k}(D) + \mathcal{A}_{1,k}(t, \mathbf{x}, D)$$

where all coefficients $a(t, \mathbf{x})$ of the operators $\mathcal{A}_{1,k}(t, \mathbf{x}, D)$ satisfy

$$\sup\Big\{|a(t,\mathbf{x})| : \ \mathbf{x} \in \mathbb{R}^n,\ t \in J_0\Big\} \leq 2\,\eta < \eta_0.$$

Therefore, corollary 3.3.1 is applicable and shows that each of these operators has maximal L_p-regularity. Furthermore, the solution operators T^k of the generalized Stokes problem for $\mathcal{A}_k$ have their norms bounded by a constant which is independent of the covering of $\mathbb{R}^n$ and of the time interval J_i for $i = 0, \dots, m-1$.

Suppose that $(\mathbf{u}, p)$ is a solution of (3.35), and let the pressure p be normalized by the condition

$$\int_{B_{2R}(0)} p(t, \mathbf{x})\, d\mathbf{x} = 0. \tag{3.44}$$

Note that this normalization of p is appropriate to apply the Poincaré inequality lemma 3.2.1 and that we may assume φ_0 to satisfy $\varphi_0 \equiv 1$ on $B_{2R}(0)^c$, hence, $\operatorname{supp}(\nabla\varphi_0) \subset \overline{B_{2R}(0)}$. Setting

$$\mathbf{u}_k := \varphi_k \mathbf{u}, \qquad p_k := \varphi_k p, \qquad g_k := \varphi_k g \quad \text{for } k = 0, \dots, N.$$

We obtain the following problem for the functions $\mathbf{u}_k$ and p_k.

$$\begin{aligned} \tfrac{\partial}{\partial t}\mathbf{u}_k + \mathcal{A}_k(t, \mathbf{x}, D)\mathbf{u}_k + \nabla p_k &= p\nabla\varphi_k + [\mathcal{A}, \varphi_k]\,\mathbf{u}, && t \in J_0, \mathbf{x} \in \mathbb{R}^n \\ \operatorname{div} \mathbf{u}_k &= g_k + (\nabla\varphi_k, \mathbf{u})\,, && t \in J_0, \mathbf{x} \in \mathbb{R}^n \\ \mathbf{u}_{k|_{t=0}} &= 0. \end{aligned}$$

Here, the commutator $[\mathcal{A}, \varphi_k]\mathbf{u}$ is defined as

$$[\mathcal{A}, \varphi_k]\mathbf{u} := \mathcal{A}(t, \mathbf{x}, D)(\varphi_k \mathbf{u}) - \varphi_k \mathcal{A}(t, \mathbf{x}, D)\mathbf{u}_k.$$

It comprises a differential operator of order 1, i.e., a lower order term. Employing the solution operator T^k, we obtain the representation

$$\begin{bmatrix} \mathbf{u}_k \\ p_k \end{bmatrix} = T^k \begin{bmatrix} (p\nabla\varphi_k) + [\mathcal{A}, \varphi_k]\mathbf{u} \\ g_k + (\nabla\varphi_k, \mathbf{u}) \end{bmatrix}.$$

Summing over all charts $k = 0, \dots, N$ this yields

$$\begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \sum_{k=0}^{N} \begin{bmatrix} \mathbf{u}_k \\ p_k \end{bmatrix} = \sum_{k=0}^{N} T^k \begin{bmatrix} (p\nabla\varphi_k) + [\mathcal{A}, \varphi_k]\mathbf{u} \\ g_k + (\nabla\varphi_k, \mathbf{u}) \end{bmatrix}.$$

We split this representation into three parts according to

$$\begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \sum_{k=0}^{N} T^k \begin{bmatrix} 0 \\ g_k \end{bmatrix} + B \begin{bmatrix} p \\ \mathbf{u} \end{bmatrix} + R\mathbf{u}, \tag{3.45}$$

where

$$B \begin{bmatrix} p \\ \mathbf{u} \end{bmatrix} = \sum_{k=0}^{N} T^k \begin{bmatrix} (p\nabla\varphi_k) \\ (\nabla\varphi_k, \mathbf{u}) \end{bmatrix} \quad \text{and} \quad R\mathbf{u} = \sum_{k=0}^{N} T^k \begin{bmatrix} [\mathcal{A}, \varphi_k]\mathbf{u} \\ 0 \end{bmatrix}.$$

In the following, we use the notation

$$X := L_p(J_0 \times \mathbb{R}^n; \mathbb{R}^n), \qquad X_p := W_p^{2-2/p}(\mathbb{R}^n; \mathbb{R}^n)$$

and

$$Y := H_p^1(J_0; \dot{H}_p^{-1}(\mathbb{R}^n)) \cap L_p(J_0; H_p^1(\mathbb{R}^n)),$$

as well as

$$Z := \left(H_p^1(J_0; L_p(\mathbb{R}^n;\mathbb{R}^n)) \cap L_p(J_0; H_p^2(\mathbb{R}^n;\mathbb{R}^n))\right) \times L_p(J_0; \dot{H}_p^1(\mathbb{R}^n)).$$

In order to estimate the part with B on the right-hand side of equation (3.45), we recall that every T^k allows a decomposition of type

$$T^k = S_0 + S_1^k$$

according to (3.42), where S_0 does not depend on k. Thus,

$$B\begin{bmatrix} p \\ \mathbf{u} \end{bmatrix} = S_0 \sum_{k=0}^{N} \begin{bmatrix} (p\nabla\varphi_k) \\ (\nabla\varphi_k, \mathbf{u}) \end{bmatrix} + \sum_{k=0}^{N} S_1^k \begin{bmatrix} (p\nabla\varphi_k) \\ (\nabla\varphi_k, \mathbf{u}) \end{bmatrix}, \tag{3.46}$$

and the first sum on the right-hand side of (3.46) is zero, since the φ_k sum up to the constant 1. Therefore,

$$B\begin{bmatrix} p \\ \mathbf{u} \end{bmatrix} = \sum_{k=0}^{N} S_1^k \begin{bmatrix} (p\nabla\varphi_k) \\ (\nabla\varphi_k, \mathbf{u}) \end{bmatrix}.$$

Employing the factorization of S_1 given in (3.42), the entries of $B(p, \mathbf{u})$ satisfy

$$\begin{aligned}
B_{11}p &= (\partial_t - \Delta)^{-1} \sum_{k=0}^{N} \widetilde{S}_{11}^k \, (-\Delta)(\partial_t - \Delta)^{-1}(p\nabla\varphi_k), \\
B_{21}p &= (-\Delta)^{-1/2} \sum_{k=0}^{N} \widetilde{S}_{21}^k \, (-\Delta)(\partial_t - \Delta)^{-1}(p\nabla\varphi_k), \\
B_{12}\mathbf{u} &= (\partial_t - \Delta)^{-1} \sum_{k=0}^{N} \widetilde{S}_{12}^k \, (-\Delta)^{1/2} \, (\nabla\varphi_k, \mathbf{u}), \\
B_{22}\mathbf{u} &= (-\Delta)^{-1/2} \sum_{k=0}^{N} \widetilde{S}_{22}^k \, (-\Delta)^{1/2} \, (\nabla\varphi_k, \mathbf{u}).
\end{aligned} \tag{3.47}$$

Since $\nabla\varphi_k$ also has a compact support for $k = 0$, it follows that $(p\nabla\varphi_k)$ belongs to $L_p(J_0; H_p^1(\mathbb{R}^n;\mathbb{R}^n))$ for all $k = 0, \ldots, N$. Since $(-\Delta)^{1/2}$ is a bounded linear operator from $H_p^1(\mathbb{R}^n)$ into $L_p(\mathbb{R}^n)$, we have

$$\left|(-\Delta)^{1/2}(p\nabla\varphi_k)\right|_{L_p(J_0\times\mathbb{R}^n;\mathbb{R}^n)} \leq C \, |(p\nabla\varphi_k)|_{L_p(J_0;H_p^1(\mathbb{R}^n;\mathbb{R}^n))}.$$

Furthermore, we infer from $\operatorname{supp}(\nabla\varphi_k) \subset \overline{B_{2R}(0)}$ for all $k = 0, \ldots, N$ and from the fact that C^∞-functions $\partial_i\varphi_k$, considered as multiplication operators, belong to $\mathcal{B}(H_p^1(\mathbb{R}^n))$ that

$$\left|(-\Delta)^{1/2}(p\nabla\varphi_k)\right|_{L_p(J_0\times\mathbb{R}^n;\mathbb{R}^n)} \leq C \, |p|_{L_p(J_0;H_p^1(B_{2R}(0)))}$$

holds. Due to the specific normalization (3.44) of the pressure p, the latter has zero mean on $B_{2R}(0)$, hence the Poincaré lemma 3.2.1 is applicable and yields

$$\left|(-\Delta)^{-1/2}(p\nabla\varphi_k)\right|_{L_p(J_0\times\mathbb{R}^n;\mathbb{R}^n)} \le C\,|\nabla p|_{L_p(J_0\times\mathbb{R}^n;\mathbb{R}^n)}\,.$$

Since

$$(-\Delta)^{-1/2}(\partial_t-\Delta)^{-1} : L_p(J_0\times\mathbb{R}^n) \to H_p^{1/2}(J_0\times\mathbb{R}^n)$$

is bounded, we obtain

$$\left|(-\Delta)(\partial_t-\Delta)^{-1}(p\nabla\varphi_k)\right|_{H_p^{1/2}(J_0;L_p(\mathbb{R}^n;\mathbb{R}^n))} \le C\,|\nabla p|_{L_p(J_0\times\mathbb{R}^n;\mathbb{R}^n)}\,.$$

By means of the Sobolev embedding $H_p^{1/2}\hookrightarrow L_{2p}$ and the Hölder inequality, this results in

$$\left|(-\Delta)(\partial_t-\Delta)^{-1}(p\nabla\varphi_k)\right|_{L_p(J_0\times\mathbb{R}^n;\mathbb{R}^n)} \le C\;h^{1/2p}\;|\nabla p|_{L_p(J_0\times\mathbb{R}^n;\mathbb{R}^n)}$$

and the constant $C\,h^{1/2p}$ can be made small by choice of $h>0$. Similarly, we have

$$\begin{aligned}\left|(-\Delta)^{1/2}\,(\nabla\varphi_k,\mathbf{u})\right|_{H_p^{1/2}(J_0;L_p(\mathbb{R}^n))} &\le |(\nabla\varphi_k,\mathbf{u})|_{H_p^{1/2}(J_0;H_p^1(\mathbb{R}^n))}\\ &\le C\;|\mathbf{u}|_{H_p^{1/2}(J_0;H_p^1(\mathbb{R}^n))}\\ &\le C\;|(\partial_t-\Delta)\mathbf{u}|_{L_p(J_0\times\mathbb{R}^n)}\end{aligned}$$

and therefore

$$\left|(-\Delta)^{1/2}\,(\nabla\varphi_k,\mathbf{u})\right|_{L_p(J_0\times\mathbb{R}^n)} \le C\;h^{1/2p}\,|(\partial_t-\Delta)\mathbf{u}|_{L_p(J_0\times\mathbb{R}^n)}\,.$$

Applying these estimates to the entries of B, given by (3.47), yields

$$\left|B\begin{bmatrix}p\\ \mathbf{u}\end{bmatrix}\right|_Z \le C\;h^{1/2p}\left|\begin{bmatrix}\mathbf{u}\\ p\end{bmatrix}\right|_Z\,.$$

In order to estimate the term $R\mathbf{u}$ from the right-hand side of equation (3.45), observe first that

$$[\mathcal{A},\varphi_k]\mathbf{u}\in H_p^{1/2}(J_0;L_p(\mathbb{R}^n;\mathbb{R}^n))\cap L_p(J_0;H_p^1(\mathbb{R}^n;\mathbb{R}^n))$$

since the commutator $[\mathcal{A},\varphi_k]$ is a differential operator of first order. Therefore,

$$\begin{aligned}|R\mathbf{u}|_Z &\le C\;|[\mathcal{A},\varphi_k]\mathbf{u}|_{L_p(J_0;L_p(\mathbb{R}^n;\mathbb{R}^n))}\\ &\le C\,h^{1/2p}\;|[\mathcal{A},\varphi_k]\mathbf{u}|_{L_{2p}(J_0;L_p(\mathbb{R}^n;\mathbb{R}^n))}\\ &\le C\,h^{1/2p}\;|\mathbf{u}|_Z\,.\end{aligned}$$

These arguments show that, choosing first $\eta>0$ and then $h>0$ sufficiently small, there is a constant $C>0$ such that

$$\left|\begin{bmatrix}\mathbf{u}\\ p\end{bmatrix}\right|_Z \le C\left(|\mathbf{f}|_X+|g|_Y+|\mathbf{u}_0|_{X_p}\right)$$

holds for every solution $(\mathbf{u}, p)$ on J_0 for given data $\mathbf{f} \in X$, $g \in Y$ and $\mathbf{u}_0 \in X_p$. Therefore, the generalized Stokes operator

$$L \in \mathcal{B}(Z; X \times Y \times X_p)$$

defined by the left-hand side of (3.35) is injective and has closed range. Hence, L is semi-Fredholm for each set of coefficients which are continuous on $J \times \mathbb{R}^n$, admit uniform limits as $|\mathbf{x}| \to \infty$ and are strongly elliptic, uniformly on $J \times (\mathbb{R}^n \cup \{\infty\})$.

Define a family of operators $\{\mathcal{A}_s(t, \mathbf{x}, D)\}_{s\in[0,1]}$ according to

$$\mathcal{A}_s(t, \mathbf{x}, D) = s\, \mathcal{A}(t, \mathbf{x}, D) + (1 - s)(-\Delta) \quad \text{for } s \in [0, 1].$$

Since the arguments given above also apply to $\mathcal{A}_s$ instead of $\mathcal{A}$, the corresponding Stokes operator L_s is injective and has closed range. Due to the continuity of the Fredholm index, the latter must be constant. Since L_0 is bijective by theorem 3.3.2, the Fredholm index of L_s is zero for all $s \in [0, 1]$. Consequently, $L = L_1$ is also surjective which finishes the proof. □

3.3.4 The Nonlinear Problem

This section provides the final step for the proof of our main result theorem 3.3.1, i.e., we consider the nonlinear problem

$$\begin{aligned} \tfrac{\partial}{\partial t}\mathbf{u} + \operatorname{div}(\mathbf{u} \otimes \mathbf{u}) &= \operatorname{div}\mathbf{S} - \nabla p + \mathbf{f}, && \text{in } t > 0, \mathbf{x} \in \mathbb{R}^n \\ \operatorname{div}\mathbf{u} &= 0, && \text{in } t > 0, \mathbf{x} \in \mathbb{R}^n \\ \mathbf{u}_{|_{t=0}} &= \mathbf{u}_0, && \text{in } \mathbb{R}^n. \end{aligned} \tag{3.48}$$

where

$$\mathbf{S} = 2\mu(\|\mathbf{D}\|^2)\mathbf{D} \quad \text{with} \quad \mathbf{D} = \frac{1}{2}\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right).$$

In the following, we assume that $\mu \in C^2(\mathbb{R}_+)$ satisfies

$$\mu(s) > 0 \quad \text{and} \quad \mu(s) + 4\left(1 - \frac{1}{n}\right) s\, \mu'(s) > 0 \quad \text{for all} \quad s \geq 0.$$

Let $p > n + 2$, fix a time interval $J_0 = [0, \tau_0]$ and let $J_\tau = [0, \tau]$ for $\tau \leq \tau_0$.

As before, we define the maximal regularity spaces

$$Z_\tau := H^1_p(J_\tau; L_p(\mathbb{R}^n; \mathbb{R}^n)) \cap L_p(J_\tau; H^2_p(\mathbb{R}^n; \mathbb{R}^n))$$

where we use the abbreviation Z_0 for Z_{τ_0}. We also set

$$X_\tau := L_p(J_\tau \times \mathbb{R}^n; \mathbb{R}^n), \qquad X_p := W^{2-2/p}_p(\mathbb{R}^n; \mathbb{R}^n),$$

and $X_0 := X_{\tau_0}$ Due to the definition of X_p as the time-trace space of Z_τ, the embedding

$$Z_\tau \hookrightarrow C(J_\tau; X_p)$$

holds, but the embedding constant blows up as $\tau \to 0+$. To circumvent this problem, it is advantageous to work with functions having a vanishing time-trace at $t = 0$. We therefore let

$$ {}_0Z_\tau := \left\{ \mathbf{u} \in Z_\tau : \mathbf{u}_{|t=0} = 0 \right\} $$

and have the embedding

$$ {}_0Z_\tau \hookrightarrow C(J_\tau; X_p), $$

where the embedding constant is uniform with respect to $\tau \in (0, \tau_0]$, see proposition 3.2.5.

In particular, since $p > n + 2$ by assumption, we have

$$ Z_\tau \hookrightarrow C(J_\tau; C^1(\mathbb{R}^n; \mathbb{R}^n)). $$

Restricted to ${}_0Z_\tau$, the uniform embedding above implies the existence of a constant $C_E > 0$ such that

$$ |\mathbf{v}|_{L_\infty(J_\tau \times \mathbb{R}^n; \mathbb{R}^n)} + |\nabla \mathbf{v}|_{L_\infty(J_\tau \times \mathbb{R}^n; \mathbb{R}^{n \times n})} \le C_E \, |\mathbf{v}|_{Z_\tau} \quad \text{for all } \mathbf{v} \in {}_0Z_\tau,\ 0 < \tau \le \tau_0. \tag{3.49} $$

At the beginning of this section, we saw that system (3.48) can be rewritten as

$$ \begin{aligned} \tfrac{\partial}{\partial t}\mathbf{u} + \mathcal{A}(\mathbf{u}, D)\mathbf{u} + \nabla p &= \mathbf{f} - \mathbf{u} \cdot \nabla \mathbf{u} && \text{in } J_\tau \times \mathbb{R}^n \\ \operatorname{div} \mathbf{u} &= 0 && \text{in } J_\tau \times \mathbb{R}^n \\ \mathbf{u}_{|t=0} &= \mathbf{u}_0 && \text{in } \mathbb{R}^n, \end{aligned} \tag{3.50} $$

The existence proof is done by reformulating the nonlinear system (3.50) as a fixed point problem in the desired regularity class, i.e., we seek for $\tau > 0$ and a fixed point of the mapping

$$ \mathbf{v} \in Z_\tau \to T\mathbf{v} := \mathbf{u} \in Z_\tau, $$

where $\mathbf{u}$ is the unique solution of the system

$$ \begin{aligned} \tfrac{\partial}{\partial t}\mathbf{u} + \mathcal{A}(\mathbf{u}_0, D)\mathbf{u} + \nabla p &= \mathbf{f} - \mathbf{v} \cdot \nabla \mathbf{v} + (\mathcal{A}(\mathbf{u}_0, D) - \mathcal{A}(\mathbf{v}, D))\,\mathbf{v} && \text{in } J_\tau \times \mathbb{R}^n \\ \operatorname{div} \mathbf{v} &= 0 && \text{in } J_\tau \times \mathbb{R}^n \\ \mathbf{v}_{|t=0} &= \mathbf{u}_0 && \text{in } \mathbb{R}^n. \end{aligned} \tag{3.51} $$

Since $\mathbf{u}_0 \in X_p$, the operator $\mathcal{A}(\mathbf{x}, D)$ results from inserting $\mathbf{u}_0$ in $\mathcal{A}(\mathbf{u}_0, D)$, i.e., $\mathcal{A}(\mathbf{x}, D) := \mathcal{A}(\mathbf{u}_0(\mathbf{x}), D)$, in fact we have $\mathcal{A}(\mathbf{x}, D) := \mathcal{A}(\nabla \mathbf{u}_0(\mathbf{x}), D)$. Then, the differential operator $\mathcal{A}(\mathbf{x}, D)$ fulfills all conditions of theorem 3.3.3.

Denote by $S : X_\tau \to Z_\tau$ the solution operator which corresponds to the left-hand side of the generalized Stokes problem (3.35) with fixed $\mathbf{u}_0$ and $g = 0$. Furthermore, we denote the right-hand side of (3.51) by $G(\mathbf{v})$. Since $G : Z_\tau \to X_\tau$, we get

$$ T := S \circ G : Z_\tau \to Z_\tau. $$

Since the initial value of the solution operator is $\mathbf{u}_0$ and in general $\mathbf{u}_0 \neq 0$, we cannot use a ball with center 0 in the fixed point argument. Recall that the embedding

$Z_\tau \hookrightarrow C(J_\tau; X_p)$ is then not uniform with respect to τ. Therefore, we choose a ball around a reference solution $\mathbf{u}^*$ in Z_τ of the linear system

$$\begin{aligned} \tfrac{\partial}{\partial t}\mathbf{u} + \mathcal{A}(\mathbf{u}_0, D)\mathbf{u} + \nabla p &= -\mathbf{u}_0 \cdot \nabla \mathbf{u}_0 && \text{in } J_\tau \times \mathbb{R}^n \\ \operatorname{div} \mathbf{u} &= 0 && \text{in } J_\tau \times \mathbb{R}^n \\ \mathbf{u}_{|t=0} &= \mathbf{u}_0 && \text{in } \mathbb{R}^n. \end{aligned}$$

We consider the mapping T on sets $K_r \subset Z_\tau$ of the form

$$K_r = \{\mathbf{u}^*\} + B_r(0) \quad \text{with} \quad B_r(0) \subset {}_0Z_\tau.$$

In order to apply the contraction mapping theorem, it has to be shown that

$$T : K_r \to K_r$$

is a contraction mapping provided that $\tau \in (0, \tau_0]$ and $r > 0$ are suitable chosen. For this purpose, we have to show the following two conditions

(i) $T(K_r) \subset K_r$

(ii) $|T(\mathbf{u}) - T(\overline{\mathbf{u}})|_{Z_\tau} \le k\,|(\mathbf{u} - \overline{\mathbf{u}})|_{Z_\tau}$ for all $\mathbf{u}, \overline{\mathbf{u}} \in K_r$ with $k < 1$.

We start with assertion (i).

Let $\overline{\mathbf{u}} \in K_r$ and $\mathbf{u} = T(\overline{\mathbf{u}})$, i.e.,

$$\begin{aligned} \tfrac{\partial}{\partial t}\mathbf{u} + \mathcal{A}(\mathbf{u}_0, D)\mathbf{u} + \nabla p &= -\overline{\mathbf{u}} \cdot \nabla \overline{\mathbf{u}} + \big(\mathcal{A}(\mathbf{u}_0, D) - \mathcal{A}(\overline{\mathbf{u}}, D)\big)\overline{\mathbf{u}} \\ \operatorname{div} \mathbf{u} &= 0 \\ \mathbf{u}_{|t=0} &= \mathbf{u}_0. \end{aligned}$$

Then, given the reference solution $\mathbf{u}^* \in Z_\tau$, we obtain

$$\begin{aligned} \big|T(\overline{\mathbf{u}}) - \mathbf{u}^*\big|_{Z_\tau} &= \big|\mathbf{u} - \mathbf{u}^*\big|_{Z_\tau} \\ &\le C_1\,|\mathbf{u}_0 \cdot \nabla \mathbf{u}_0 - \overline{\mathbf{u}} \cdot \nabla \overline{\mathbf{u}}|_{X_\tau} + C_1\,\big|\big(\mathcal{A}(\mathbf{u}_0, D) - \mathcal{A}(\overline{\mathbf{u}}, D)\big)\overline{\mathbf{u}}\big|_{X_\tau} \end{aligned} \tag{3.52}$$

The two terms of the right-hand side of inequality (3.52) are treated separately. Starting with the first one, we obtain the estimate

$$\big|\mathbf{u}_0 \cdot \nabla \mathbf{u}_0 - \overline{\mathbf{u}} \cdot \nabla \overline{\mathbf{u}}\big|_{X_\tau} \le \big|(\mathbf{u}_0 - \overline{\mathbf{u}}) \cdot \nabla \mathbf{u}_0\big|_{X_\tau} + \big|\overline{\mathbf{u}} \cdot \nabla (\mathbf{u}_0 - \overline{\mathbf{u}})\big|_{X_\tau} \tag{3.53}$$

For the first term of the right-hand side of inequality (3.53) we get

$$\begin{aligned} \big|(\mathbf{u}_0 - \overline{\mathbf{u}}) \cdot \nabla \mathbf{u}_0\big|_{X_\tau} &\le |\nabla \mathbf{u}_0|_{L_\infty(J_\tau \times \mathbb{R}^n; \mathbb{R}^{n\times n})}\,\big|\mathbf{u}_0 - \overline{\mathbf{u}}\big|_{X_\tau} \\ &\le C\big|\mathbf{u}_0 - \overline{\mathbf{u}}\big|_{X_\tau} \\ &\le C\,\tau^{1/p}\,|\mathbf{u}_0 - \overline{\mathbf{u}}|_{L_\infty(J_\tau; L_p(\mathbb{R}^n; \mathbb{R}^n))} \\ &\le C\,\tau^{1/p}\big|\mathbf{u}_0 - \overline{\mathbf{u}}\big|_{Z_\tau} \\ &\le C\,\tau^{1/p}\Big(\big|\mathbf{u}_0 - \mathbf{u}^*\big|_{Z_\tau} + r\Big) \\ &\le C\,\tau^{1/p} \to 0+ \quad \text{as} \quad \tau \to 0+ \end{aligned} \tag{3.54}$$

in case $r \leq 1$, say. In the estimate above, the letter C denotes different constants from line to line. For the second term of the right-hand side of inequality (3.53), using inequality (3.49), we infer

$$\begin{aligned}
\big|\overline{\mathbf{u}} \cdot \nabla(\mathbf{u}_0 - \overline{\mathbf{u}})\big|_{X_\tau} &\leq |\overline{\mathbf{u}}|_{X_\tau} \, |\nabla(\mathbf{u}_0 - \overline{\mathbf{u}})|_{L_\infty(J_\tau \times \mathbb{R}^n; \mathbb{R}^{n\times n})} \\
&\leq C_E \big|\overline{\mathbf{u}}\big|_{X_\tau} \big|\mathbf{u}_0 - \overline{\mathbf{u}}\big|_{Z_\tau} \\
&\leq C_E \, \tau^{1/p} \, |\overline{\mathbf{u}}|_{L_\infty(J_\tau; L_p(\mathbb{R}^n; \mathbb{R}^n))} \Big(\big|\mathbf{u}_0 - \mathbf{u}^*\big|_{Z_\tau} + r \Big) \\
&\leq C \, \tau^{1/p} \big|\overline{\mathbf{u}}\big|_{Z_\tau} \Big(\big|\mathbf{u}_0 - \mathbf{u}^*\big|_{Z_\tau} + r \Big) \\
&\leq C \, \tau^{1/p} \Big(\big|\mathbf{u}^*\big|_{Z_\tau} + r \Big) \Big(\big|\mathbf{u}_0 - \mathbf{u}^*\big|_{Z_\tau} + r \Big) \\
&\leq C \, \tau^{1/p} \to 0+ \quad \text{as} \quad \tau \to 0+ \,. \qquad (3.55)
\end{aligned}$$

Next, we consider the second term of the right-hand side of inequality (3.52). For this purpose, we define $\mathbf{D}^0 := \mathbf{D}(\mathbf{u}_0) = 1/2 \left[\nabla \mathbf{u}_0 + (\nabla \mathbf{u}_0)^T\right]$ and $\mathbf{D}^0 = (d^0_{ij})$, further let $\overline{\mathbf{D}}$ be analogously given by $\overline{\mathbf{D}} := (\overline{d}_{ij})$.

Then, we have

$$\begin{aligned}
\big|\big(\mathcal{A}(\mathbf{u}_0, D) - \mathcal{A}(\overline{\mathbf{u}}, D)\big)\overline{\mathbf{u}}\big|_{X_\tau} &\leq \big|\mu(\|\mathbf{D}^0\|^2) \Delta \overline{\mathbf{u}} - \mu(\|\overline{\mathbf{D}}\|^2) \Delta \overline{\mathbf{u}}\big|_{X_\tau} \\
&\quad + 4 \left| \sum_{k,l=1}^n \big(\mu'(\|\mathbf{D}^0\|^2) d^0_{ik} d^0_{jl} - \mu'(\|\overline{\mathbf{D}}\|^2) \overline{d}_{ik} \overline{d}_{jl}\big) \, D_k D_l \overline{\mathbf{u}} \right|_{X_\tau} \\
&\leq \big|\mu(\|\mathbf{D}^0\|^2) - \mu(\|\overline{\mathbf{D}}\|^2)\big|_{L_\infty(J_\tau \times \mathbb{R}^n)} \big|\Delta \overline{\mathbf{u}}\big|_{X_\tau} \\
&\quad + 4 \sum_{k,l=1}^n \big|\mu'(\|\mathbf{D}^0\|^2) d^0_{ik} d^0_{jl} - \mu'(\|\overline{\mathbf{D}}\|^2) \overline{d}_{ik} \overline{d}_{jl}\big|_{L_\infty(J_\tau \times \mathbb{R}^n)} \big|\overline{\mathbf{u}}\big|_{Z_\tau}
\end{aligned}$$

For large $R > 0$ is $\big\|\mathbf{D}^0\big\|^2, \big\|\overline{\mathbf{D}}\big\|^2 < R$ a.e. on $J_\tau \times \mathbb{R}^n$ and by assumption μ, μ' are

Lipschitz continuous with a joint constant $L > 0$ on $[0, R]$. It follows that

$$\begin{aligned}
\big|\big(\mathcal{A}(\mathbf{u}_0, D) - \mathcal{A}(\overline{\mathbf{u}}, D)\big)\overline{\mathbf{u}}\big|_{X_\tau} &\le L\Big|\|\mathbf{D}^0\|^2 - \|\overline{\mathbf{D}}\|^2\Big|_{L_\infty(J_\tau\times\mathbb{R}^n)}\big|\overline{\mathbf{u}}\big|_{Z_\tau} \\
&\quad + C\sum_{k,l=1}^n \big|d_{ik}^0 d_{jl}^0 - \overline{d}_{ik}\overline{d}_{jl}\big|_{L_\infty(J_\tau\times\mathbb{R}^n)}\big|\overline{\mathbf{u}}\big|_{Z_\tau} \\
&\quad + 4\sum_{k,l=1}^n \Big|\Big(\mu'(\|\mathbf{D}^0\|^2) - \mu'(\|\overline{\mathbf{D}}\|^2)\Big)\overline{d}_{ik}\overline{d}_{jl}\Big|_{L_\infty(J_\tau\times\mathbb{R}^n)}\big|\overline{\mathbf{u}}\big|_{Z_\tau} \\
&\le L\Big|\,\|\mathbf{D}^0\| - \|\overline{\mathbf{D}}\|\,\Big|_{L_\infty(J_\tau\times\mathbb{R}^n)}\Big|\,\|\mathbf{D}^0\| + \|\overline{\mathbf{D}}\|\,\Big|_{L_\infty(J_\tau\times\mathbb{R}^n)}\big|\overline{\mathbf{u}}\big|_{Z_\tau} \\
&\quad + C\sum_{k,l=1}^n \Big(\big|d_{ik}^0\big|_{L_\infty(J_\tau\times\mathbb{R}^n)}\big|d_{jl}^0 - \overline{d}_{jl}\big|_{L_\infty(J_\tau\times\mathbb{R}^n)} + \\
&\qquad\qquad \big|d_{ik}^0 - \overline{d}_{ik}\big|_{L_\infty(J_\tau\times\mathbb{R}^n)}\big|\overline{d}_{jl}\big|_{L_\infty(J_\tau\times\mathbb{R}^n)}\Big)\big|\overline{\mathbf{u}}\big|_{Z_\tau} \\
&\quad + 4L\sum_{k,l=1}^n \big|\overline{d}_{ik}\overline{d}_{jl}\big|_{L_\infty(J_\tau\times\mathbb{R}^n)}\Big|\|\mathbf{D}^0\|^2 - \|\overline{\mathbf{D}}\|^2\Big|_{L_\infty(J_\tau\times\mathbb{R}^n)}\big|\overline{\mathbf{u}}\big|_{Z_\tau} \\
&\le C\Big|\nabla(\mathbf{u}_0 - \overline{\mathbf{u}})\Big|_{L_\infty(J_\tau\times\mathbb{R}^n;\mathbb{R}^{n\times n})}\big|\overline{\mathbf{u}}\big|_{Z_\tau} \\
&\le C\Big|\nabla(\mathbf{u}_0 - \overline{\mathbf{u}})\Big|_{L_\infty(J_\tau\times\mathbb{R}^n;\mathbb{R}^{n\times n})}\Big(\big|\mathbf{u}^*\big|_{Z_\tau} + r\Big) \qquad (3.56)
\end{aligned}$$

and

$$\Big|\nabla(\mathbf{u}_0 - \overline{\mathbf{u}})\Big|_{L_\infty(J_\tau\times\mathbb{R}^n;\mathbb{R}^{n\times n})} \to 0 \quad \text{as } \tau \to 0+,$$

due to $\overline{\mathbf{u}} \in C(J_0; C^1(\mathbb{R}^n))$ with $\nabla\overline{\mathbf{u}}(t,\cdot) \to \nabla\mathbf{u}_0$ in $L_\infty(\mathbb{R}^n;\mathbb{R}^{n\times n})$ as $t \to 0+$.

Thus, combining the results (3.54)-(3.56) we obtain that T is a self-mapping of Z_τ. As next, we prove assertion (ii). Given $\mathbf{u}, \overline{\mathbf{u}} \in K_r$, then

$$\begin{aligned}
\big|T(\mathbf{u}) - T(\overline{\mathbf{u}})\big|_{Z_\tau} &\le \big|\overline{\mathbf{u}}\cdot\nabla\overline{\mathbf{u}} - \mathbf{u}\nabla\mathbf{u}\big|_{X_\tau} + \big|\left(\mathcal{A}(\mathbf{u}_0, D) - \mathcal{A}(\overline{\mathbf{u}}, D)\right)(\mathbf{u} - \overline{\mathbf{u}})\big|_{X_\tau} \\
&\quad + \big|\left(\mathcal{A}(\overline{\mathbf{u}}, D) - \mathcal{A}(\mathbf{u}, D)\right)\mathbf{u}\big|_{X_\tau} \qquad (3.57)
\end{aligned}$$

Once more, we treat the arising terms in inequality (3.57) separately. For the first term we receive in analogy to estimate (3.53), respectively (3.54) and (3.55), the following estimate

$$\begin{aligned}
&\big|\overline{\mathbf{u}}\cdot\nabla\overline{\mathbf{u}} - \mathbf{u}\cdot\nabla\mathbf{u}\big|_{X_\tau} \\
&\quad\le |\nabla\overline{\mathbf{u}}|_{L_p(J_\tau\times\mathbb{R}^n;\mathbb{R}^{n\times n})}|\overline{\mathbf{u}} - \mathbf{u}|_{L_\infty(J_\tau\times\mathbb{R}^n;\mathbb{R}^n)} + \big|\mathbf{u}\big|_{X_\tau}|\nabla(\overline{\mathbf{u}} - \mathbf{u})|_{L_\infty(J_\tau\times\mathbb{R}^n;\mathbb{R}^{n\times n})} \\
&\quad\le C\left(|\nabla\overline{\mathbf{u}}|_{L_p(J_\tau\times\mathbb{R}^n;\mathbb{R}^{n\times n})} + \big|\mathbf{u}\big|_{X_\tau}\right)\big|\overline{\mathbf{u}} - \mathbf{u}\big|_{Z_\tau} \\
&\quad\le C\tau^{1/p}\left(|\nabla\overline{\mathbf{u}}|_{L_\infty(J_\tau;L_p(\mathbb{R}^n;\mathbb{R}^{n\times n}))} + |\mathbf{u}|_{L_\infty(J_\tau;L_p(\mathbb{R}^n;\mathbb{R}^n))}\right)\big|\overline{\mathbf{u}} - \mathbf{u}\big|_{Z_\tau} \\
&\quad\le C\tau^{1/p}\left(\big|\mathbf{u}^*\big|_{Z_\tau} + r\right)\big|\overline{\mathbf{u}} - \mathbf{u}\big|_{Z_\tau}
\end{aligned}$$

In analogy to estimate (3.56), the second term of the right-hand side of inequality (3.57) results in

$$\begin{aligned}\left| \left(\mathcal{A}(\mathbf{u}_0, D) - \mathcal{A}(\overline{\mathbf{u}}, D)\right)(\mathbf{u} - \overline{\mathbf{u}})\right|_{X_\tau} &\leq C\,|\nabla(\mathbf{u}_0 - \overline{\mathbf{u}})|_{L_\infty(J_\tau \times \mathbb{R}^n; \mathbb{R}^{n\times n})}\left|\mathbf{u} - \overline{\mathbf{u}}\right|_{Z_\tau} \\ &\leq C\left|\mathbf{u}_0 - \overline{\mathbf{u}}\right|_{Z_\tau}\left|\mathbf{u} - \overline{\mathbf{u}}\right|_{Z_\tau} \\ &\leq C\left(\left|\mathbf{u}_0 - \mathbf{u}^*\right|_{Z_\tau} + r\right)\left|\mathbf{u} - \overline{\mathbf{u}}\right|_{Z_\tau}\end{aligned}$$

and the third term yields

$$\begin{aligned}\left| \left(\mathcal{A}(\overline{\mathbf{u}}, D) - \mathcal{A}(\mathbf{u}, D)\right)\mathbf{u}\right|_{X_\tau} &\leq C\,|\nabla(\overline{\mathbf{u}} - \mathbf{u})|_{L_\infty(J_\tau \times \mathbb{R}^n; \mathbb{R}^{n\times n})}\left|\mathbf{u}\right|_{Z_\tau} \\ &\leq C\left(\left|\mathbf{u}^*\right|_{Z_\tau} + r\right)\left|\overline{\mathbf{u}} - \mathbf{u}\right|_{Z_\tau}.\end{aligned}$$

Now, fix $r \leq (0, 1]$ such that $r \leq 1/8C$ and $\tau \in (0, \tau_0]$ such that

$$\left|\mathbf{u}^* - \mathbf{u}_0\right|_{Z_\tau} \leq r, \qquad \left|\mathbf{u}^*\right|_{Z_\tau} \leq r.$$

If, in addition, τ is chosen so small that $\tau^{1/p} \leq 1/4C$, then

$$\left|T(\mathbf{u}) - T(\overline{\mathbf{u}})\right|_{Z_\tau} \leq \frac{3}{4}\left|\mathbf{u} - \overline{\mathbf{u}}\right|_{Z_\tau}.$$

Thus, T is a strict contraction.

Therefore, we obtain via the contraction mapping principle a unique solution of system (3.50) in the maximal L_p-regularity class. Hence, theorem 3.3.1 is proven.

3.4 Related Work

In this section we give a short survey about related mathematical literature. In particular, existence and uniqueness results for system (3.2) are studied for bounded smooth domains $\Omega \subset \mathbb{R}^n$. The following initial-boundary problem is investigated,

$$\begin{aligned}\tfrac{\partial}{\partial t}\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} &= \operatorname{div}\mathbf{S} - \nabla p + \mathbf{f}, && \text{in } J\times\Omega \\ \operatorname{div}\mathbf{u} &= 0, && \text{in } J\times\Omega \\ \mathbf{u}_{|_{t=0}} &= \mathbf{u}_0, && \text{in } \Omega \\ &\text{with boundary condition on } \partial\Omega.\end{aligned} \tag{3.58}$$

Especially, many authors prove existence results for the *Dirichlet* and the *space periodic* problem, respectively. In case of the Dirichlet problem the usually Dirichlet condition

$$\mathbf{u}_{|_{\partial\Omega}} = 0, \text{ on } \partial\Omega,$$

is required at the boundary, whereas in case of the space-periodic problem, Ω is considered as a cube in $\mathbb{R}^n$ and for $(\mathbf{u}, p)$ periodicity on the boundary of Ω is assumed. In the following we turn to these main areas of interest. However, there are also some results for Neumann boundary conditions [Zad96].

In general, the following model problems [MNR01] are often considered for $m > 0$ and the zero-shear viscosity $\mu_0 > 0$,

$$\begin{aligned}
(a) \quad \mathbf{S}(\mathbf{D}) &= 2\mu_0 \|\mathbf{D}\|^{m-2}\mathbf{D} \\
(b) \quad \mathbf{S}(\mathbf{D}) &= 2\mu_0\big(1+\|\mathbf{D}\|^2\big)^{\frac{m-2}{2}}\mathbf{D} \\
(c) \quad \mathbf{S}(\mathbf{D}) &= 2\mu_0\big(1+\|\mathbf{D}\|\big)^{m-2}\mathbf{D} \\
(d) \quad \mathbf{S}(\mathbf{D}) &= 2\mu_0\big(1+\|\mathbf{D}\|^{m-2}\big)\mathbf{D},
\end{aligned}$$

where $\|\mathbf{D}\|$ denotes the Frobenius norm. All these models have some joint properties:

- for $m = 2$ all formulas reduce to the Newtonian case $\mu(\dot\gamma) = \mu_0$,
- for all models a scalar potential can be constructed,
- they satisfy the coercivity condition $\mathbf{S}\cdot\mathbf{D} \geq 2\mu_0\|\mathbf{D}\|^m$,
- they have $(m-1)$ growth, which means $|\mathbf{S}| \leq c(1+\|\mathbf{D}\|)^{m-1},\ c > 0$.

Despite their similar structure, the asymptotic behavior of the viscosity function $\mu(s)$ as $s \to 0+$ or $s \to \infty$ differ extremely [MNRR96], [MNR01]. Thus, these models enclose a multitude of physical problems.

In this context, the question arises: for which exponents m does a strong solution exist. We emphasize that according to the engineering literature, the range of interest concerning m is $m > 1$. With respect to section 2.5, we mention that the effect of shear thinning is described for $1 < m < 2$ and the effect of shear thickening for $m > 2$.

The first mathematical investigations of system (3.58) with Dirichlet boundary condition go back to Ladyzhenskaya [Lad69]. She proved existence of weak solutions to all models (a)–(d) for $m \geq 1 + 2n/(n+2)$ and their uniqueness for $m \geq (n+2)/2$, where n denotes the space dimension. Many existence results base on Malek, Necas and Ruzicka [MNR93] and Bellout, Bloom, and Necas [BBN94]. A detailed discussion of existence results for generalized Newtonian fluids can be found in the monograph [MNRR96], a historical overview is also included in [MNR01].

Amann [Ama94], [Ama99] showed existence ($n = 3$) of a classical solutions for small data $\mathbf{f}$ and $\mathbf{u}_0$ and under the assumption that $\partial_{kl}\mathbf{S}(\mathbf{0}) = \text{const.} > 0$. For the models (b) and (c), Amann obtained existence if $m \geq 1$ and for model (d) if $m \geq 2$. In fact, Amann investigated the more general case $\mathbf{S} = \alpha_1\mathbf{D} + \alpha_2\mathbf{D}^2$, where the scalar functions α_1, α_2 depend on the principal tensor invariants of $\mathbf{D}$. In this paper the energy conservation equation is also included.

Malek, Necas, and Ruzicka [MNR01] were able to show the existence of weak solutions for $m \geq 2$ in the 3 dimensional space and if $m \geq 9/4$ then a weak solution is strong and unique among all weak solutions, assuming that the stress tensor $\mathcal{S}$ is more or less given in the form of the standard example and satisfies restrictive coercivity conditions. Furthermore, Frehse, Màlek, and Steinhauer showed existence of weak solutions for stationary flows with Dirichlet boundary condition for $m > 2n/(n+2)$, $n \geq 2$ [FMS97], [FMS03].

We turn to existence results for the space periodic problem. In [MRR95], Màlek, Rajagopal, and Ruzicka proved existence of weak solutions for $m \in (3n/(n+2), 2n/(d-2))$ and uniqueness of weak solutions for $m \geq (3n+2)/(n+2)$. Global strong solutions for small data are obtained in [MRR95] and [MNRR96] for $m \geq (3n-4)/n$.

Error analysis for a fully implicit space time discretization of an unsteady, non-Newtonian fluid flow model can be found in [PR01].

Strong solutions were already obtained in Màlek, Necas, and Ruzicka [MNR93] under the assumption $m \geq 1$ in 2D and $m \geq (3n+2)/(n+2)$, $n \geq 3$. In [MNRR96], an existence result for strong solutions for small times for $m > 5/3$ is given, which has recently been extended to $m > 7/5$ in $3D$ by Diening and Ruzicka [DR03], [Die02], [DPR02]. For $7/5 < m \leq 2$ Diening and Ruzicka obtain for the regularity of the velocity field $u \in C([0;T]; W^{1,6(m-1)-\varepsilon}_{\mathrm{div}}(\Omega))$ for all $\varepsilon > 0$, where $W^{k,q}_{\mathrm{div}}(\Omega)$ denotes the closure of $\{\phi \in C^\infty_{\mathrm{per}} : \ \mathrm{div}\,\phi = 0, \langle \phi, 1\rangle = 0\}$ with respect to the $|\cdot|_{k,q}$-norm. Within this class of regularity, they prove uniqueness for all $m > 7/5$.

In order to compare our existence result with the literature, recall that for the space dimension n theorem 3.3.1 provides local existence in the maximal regularity class if the viscosity function fulfills the following two conditions

$$\mu(s) \ > \ 0 \tag{3.59-a}$$

$$\mu(s) + 4\left(1 - \frac{1}{n}\right) s\,\mu'(s) \ > \ 0. \tag{3.59-b}$$

Thus, we get for the standard example (b), given by $\mu(s) = (1+s)^{\frac{m-2}{2}}$, that condition (3.59-a) is obviously satisfied and condition (3.59-b) yields

$$\mu(s)\left[1 + C\left(2 - \frac{2}{n}\right)(m-2)\right] > 0 \text{ with } C := \frac{s}{1+s}.$$

Therefore, we obtain existence for

$$m > 2 - \frac{n}{C(2n-2)}.$$

Due to $0 \leq C < 1$, we get the worst case for $C = 1$. Hence, local existence in the maximal regularity class is obtained for

$$m > \frac{3n-4}{2(n-1)}.$$

Thus, in the 3D case a value of $m > 5/4$ is sufficient.

Furthermore, we recall some important results concerning the solvability of the generalized Stokes equations with variable coefficients. In [Sol01b], Solonnikov consider the system

$$\begin{array}{rcll} \frac{\partial}{\partial t}\mathbf{u} + A(t,\mathbf{x},\frac{\partial}{\partial x}) + \nabla p & = & \mathbf{f}, & \text{for } \mathbf{x} \in \Omega \subset \mathbb{R}^3,\ t \in (0,T) \\ \mathrm{div}\,\mathbf{u} & = & 0 & \\ \mathbf{u}(0,\mathbf{x}) = \mathbf{u}_0(\mathbf{x}), & & \mathbf{u}(t,\mathbf{x})_{|_{\mathbf{x}\in\partial\Omega}} = a(t,\mathbf{x}) & \end{array} \tag{3.60}$$

where A is a matrix elliptic-type differential operator with real coefficients depending on t and $\mathbf{x}$. Under certain assumptions on the data, Solonnikov proved the solvability of problem (3.60) in anisotropic Sobolev spaces. In [Sol01a], Solonnikov consider system (3.60) with $a(t, \mathbf{x}) = 0$ and showed that the problem has a unique solution in Hölder spaces. The generalized Stokes equations with constant coefficients in the half-space is studied by Solonnikov in [Sol01c]. The latter result is used in the proof of problem (3.60), [Sol01b].

Chapter 4

Numerical Analysis of Two-phase Flows

In this chapter some fundamental concepts solving the Navier-Stokes system numerically are discussed, such as the finite volume method and the Chorin method [CM79], [GR96]. Then, we turn to two-phase flow, since many interesting problems appear in this context. A survey of the physical features of two-phase flow modeling is presented and especially the treatment of the interface is discussed. Since we employ the volume of fluid (VOF) method for description of the interface, one section deals with the surface tension regarding spurious currents.

In chapter 2 the different behavior of non-Newtonian fluids were described and generalized Newtonian fluids were introduced. Starting from this class of models, it was shown under which circumstances these models admit a local strong solution in their maximal regularity class within L_p-setting. Here, we consider the numerical treatment of these models. Further on, the numerical simulations are compared with the physical experiment of a binary droplet collision, based on our paper [MRB$^+$02].

All numerical investigations are based on the massively parallelized VOF-code *FS3D* (Free Surface 3D). This program was developed at the University Stuttgart (ITLR, Germany) [RF99] and further developments were done in a joint project of PC^2 and the Technische Chemie (chemical engineering) at University Paderborn. A detailed description of the program *FS3D* and the used methods is given in [Rie04]. Results about an ultrasonic atomization calculated with *FS3D* are presented in [Rei02], [RBM$^+$02], [Les04], and [BLRW04]. Further simulation results concerning bubble flows are given in [KBPW02], [KBW03], [BKW04a] and concerning mass transfer in [BKWW03], [BKW$^+$04b], [Koe04].

To complete this chapter, we quote an existence result of Escher, Prüss, and Simonett [EPS03] for the two-phase Navier-Stokes system. We continue to use the notations of chapter 2.

4.1 Numerical Treatment of the Navier-Stokes Equations

4.1.1 Boundary Conditions

So far, we investigated the Navier-Stokes system in the whole space $\mathbb{R}^n$, whereas in the numerical context we are restricted to flows in bounded domains $\Omega \subset \mathbb{R}^n$. In such cases, we have to require conditions on the boundary in order to achieve a unique solution of the differential system which in its conservative formulation is given by

$$\begin{aligned} \frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) &= \operatorname{div} \mathbf{S} - \nabla p + \rho \mathbf{f}, && \text{in } J \times \Omega \\ \operatorname{div} \mathbf{u} &= 0, && \text{in } J \times \Omega \\ \mathbf{u}_{|t=0} &= \mathbf{u}_0, && \text{in } \Omega \end{aligned} \tag{4.1}$$

with the stress tensor $\mathbf{S} = 2\ \mu(\|\mathbf{D}\|^2)\mathbf{D}$, the deformation tensor $\mathbf{D} = \frac{1}{2}\left[\nabla \mathbf{u} + (\nabla \mathbf{u})^T\right]$, and the shear rate $\dot{\gamma} = \sqrt{2\ \operatorname{tr}(\mathbf{D}^2)}$.

Depending on the physical situation, different boundary conditions occur. Especially, we distinguish between Dirichlet and Neumann boundary conditions. The Dirichlet boundary condition prescribes the value of the velocity on the boundary, whereas the Neumann condition prescribes the gradient of the velocity perpendicular to the boundary.

The decomposition of the velocity $\mathbf{u}$ in its normal component $u^N := \mathbf{u} \cdot \mathbf{n}$ and its tangential part $u^T := \mathbf{u} - u^N \mathbf{n}$ enables the description of five different types of boundary conditions [GDN95].

(i) *No-slip* boundary conditions. The boundary ∂V is a rigid wall, i.e., no fluid comes out of the wall and the fluid adhere at the wall. On the boundary holds

$$\mathbf{u} = 0.$$

(ii) *Free-slip* boundary conditions. No fluid comes out of the wall, but in contrast to the no-slip condition, no friction acts along the wall. Therefore, we prescribe on the boundary

$$u^N = 0 \quad \text{and} \quad \boldsymbol{\tau} \cdot \mathbf{S} \cdot \mathbf{n} = 0 \text{ for each } \boldsymbol{\tau} \perp \mathbf{n}.$$

(iii) *Inflow* boundary conditions. In this case all velocity components are prescribed, i.e.,

$$\mathbf{u} = \mathbf{u}_{\text{in}}, \qquad \text{where } \mathbf{u}_{\text{in}} \text{ is given.}$$

(iv) *Outflow* boundary conditions. In order to prescribe boundary conditions at the outlet, many technics exists. Great practicable importance have the so-called "do-nothing" method [HRT96], which is of type

$$\nabla \mathbf{u} \cdot \mathbf{n} - p\, \mathbf{n} = 0$$

with a prescribed normalized pressure p.

(v) *Periodic* boundary conditions. In case of a one-directional periodical problem with periodic length π, it is sufficient to compute the solution on one period. Then, the velocities and the pressure have to be equal on both sides of the periodical direction. If we assume that the problem is periodic in the x_1 direction, it follows that

$$\begin{aligned} \mathbf{u}(0, x_2, \ldots, x_n) &= \mathbf{u}(\pi, x_2, \ldots, x_n), \\ \partial_{x_1}\mathbf{u}(0, x_2, \ldots, x_n) &= \partial_{x_1}\mathbf{u}(\pi, x_2, \ldots, x_n), \\ p(0, x_2, \ldots, x_n) &= p(\pi, x_2, \ldots, x_n). \end{aligned}$$

If the velocity is prescribed on the whole boundary of the domain, i.e. we have pure Dirichlet boundary conditions, the additional condition

$$\int_{\partial V} \mathbf{u} \cdot \mathbf{n} \, dA = 0$$

must be satisfied because the velocity field is divergence-free.

4.1.2 General Time Splitting Technique

Solving the Navier-Stokes equations numerically, the problem has to be transformed from a continuous problem into a discrete one which is considered at finite points. For the sake of better readability, we assume a Cartesian grid of equidistant width, and the investigated time interval $J = [0, T]$ is decomposed into equidistant time steps δt, thus $t_n = n\,\delta t$. In order to label the approximation of a function ϕ at the point of time t_n, we use a superscript index n, i.e., $\phi^n := \phi(t_n)$.

The most common strategy to solve the Navier-Stokes equations numerically is based on operator splitting methods, i.e., the system (4.1) is split into a series of simpler equations. In order to illustrate this strategy, we consider the simple case of a linear differential equation

$$\begin{aligned} \tfrac{d}{dt}u(t) + (A+B)u(t) &= 0, \qquad t \geq 0, \\ u(0) &= u_0 \end{aligned} \tag{4.2}$$

where A and B are constant matrices. On the assumption that we have an approximation u^n of u at time t_n, we want to compute u^{n+1}. The simplest procedure consists of two steps [GR96]. In a first step, the linear initial value problem is solved

$$\begin{aligned} \tfrac{d}{dt}u(t) + Au(t) &= 0, \qquad t \in (t_n, t_{n+1}) \\ u(t_n) &= u^n. \end{aligned} \tag{4.3}$$

We get the solution $u(t_{n+1}) = e^{-\delta t A}u^n$ and define $\tilde{u}^{n+1} := u(t_{n+1})$.

In the second step, the linear differential equation for the matrix B with the initial value $\tilde{u}^{n+1}$ is solved, i.e.,

$$\begin{aligned} \tfrac{d}{dt}u(t) + Bu(t) &= 0, \qquad t \in (t_n, t_{n+1}) \\ u(t_n) &= \tilde{u}^{n+1}. \end{aligned} \tag{4.4}$$

Thus, the solution of system (4.2) is obtained as

$$u^{n+1} = e^{-\delta t B}\tilde{u}^{n+1} = e^{-\delta t B}e^{-\delta t A}u^n,$$

in dependence of u^n. Finally, by iteration we obtain the solution dependent on the initial value u_0,

$$u^{n+1} = \left(e^{-\delta t B}e^{-\delta t A}\right)^n u_0,$$

whereas the exact solution of the discretized (with respect to t) form of the initial problem (4.2) is given by

$$u^{n+1} = \left(e^{-\delta t (A+B)}\right)^n u_0.$$

If the matrices A and B do not commute, comparison of the Taylor series of $e^{-\delta t(A+B)}$ with the product of the Taylor series of $e^{-\delta t B}$ and $e^{-\delta t A}$ shows that the two-step scheme is only first-order accurate [GR96]. The convergence of this scheme is obtained by the application of Trotter-Kato product formula

$$e^{t(A+B)} = \lim_{n\to\infty}\left(e^{tA/n}e^{tB/n}\right)^n,$$

which holds for arbitrary generators A, B of strongly continuous semigroups in a Banach space [Tro59].

A scheme of second-order accuracy can be achieved by a three step method: solving (4.3) during half of a time step, then (4.4) on a time step, and finally (4.3) on a half time step. For more details about the three step method and convergence results we refer to [GR96].

In the Navier-Stokes equations, the pressure term ∇p additionally appears. The incompressibility condition $\operatorname{div}\mathbf{u} = 0$ couples both the velocity field $\mathbf{u}$ and the pressure p. Solving this coupled system directly requires high computational effort. In order to avoid this, the classical projection method of Chorin [Cho68] can be used. The idea of this method is to decouple the calculation of the actual velocity field $\mathbf{u}$ and the pressure p at each iteration step. The projection method is illustrated for the partial differential equations

$$\begin{array}{c} \frac{\partial}{\partial t}\mathbf{u}(t,\mathbf{x}) + A\mathbf{u}(t,\mathbf{x}) + \nabla p(t,\mathbf{x}) = 0, \quad \operatorname{div}\mathbf{u} = 0, \\ \mathbf{u}(t_n,\mathbf{x}) = \mathbf{u}^n(\mathbf{x}), \qquad \mathbf{u}(t,\mathbf{x})_{|\partial\Omega} = 0 \end{array} \tag{4.5}$$

with the constant matrix A and for $t \in (t_n, t_{n+1})$, $\mathbf{x} \in \mathbb{R}^n$. At first, we solve

$$\frac{\partial}{\partial t}\mathbf{u}(t,\mathbf{x}) = -A\mathbf{u}(t,\mathbf{x}), \quad \mathbf{u}(t_n,\mathbf{x}) = \mathbf{u}^n(\mathbf{x}), \quad \mathbf{u}(t,\mathbf{x})_{|\partial\Omega} = 0$$

and denote the solution as $\tilde{\mathbf{u}}^{n+1}(\mathbf{x})$.

Given $\tilde{\mathbf{u}}^{n+1}(\mathbf{x})$, the tuple $(\mathbf{u}^{n+1}, p^{n+1})$ has to be determined as the solution of

$$\frac{1}{\delta t}\left(\mathbf{u}^{n+1} - \tilde{\mathbf{u}}^{n+1}\right) + \nabla p^{n+1} = 0, \tag{4.6-a}$$

$$\operatorname{div}\mathbf{u}^{n+1} = 0, \tag{4.6-b}$$

$$\mathbf{u}^{n+1}_{|\partial\Omega} = 0, \tag{4.6-c}$$

where an explicit Euler discretization for the time derivative $\frac{\partial}{\partial t}\mathbf{u}$ is used.

System (4.6) can be reformulated as a problem solely for the pressure function p. To achieve this, we apply the divergence on equation (4.6-a), taking into account the divergence-free condition (4.6-b) of the desired velocity field $\mathbf{u}^{n+1}$. This results in the Poisson equation for the pressure function,

$$\Delta p^{n+1} = \frac{1}{\delta t} \operatorname{div} \tilde{\mathbf{u}}^{n+1}, \qquad \nabla p^{n+1} \cdot \mathbf{n}|_{\partial\Omega} = 0. \tag{4.7}$$

In order to solve the Poisson equation (4.7) for p^{n+1}, we must prescribe Dirichlet or Neumann boundary conditions for the pressure. If the Neumann boundary condition is used as stated in (4.7), the boundary condition (4.6-c) is additionally required. This can be seen by multiplying equation (4.6-a) with the normal vector $\mathbf{n}$ and integrating over $\partial\Omega$ with respect to

$$0 = \int_\Omega \operatorname{div} \tilde{\mathbf{u}}^{n+1} \, d\mathbf{x} = \int_{\partial\Omega} \tilde{\mathbf{u}}^{n+1} \cdot \mathbf{n} \, dA.$$

is fulfilled. Then, the solution p^{n+1} is determined up to an additive constant. In order to fix the pressure p^{n+1}, it is common to require

$$\int_\Omega p^{n+1} \, d\mathbf{x} = 0.$$

In order to solve the Poisson equation different methods can be used, e.g., multigrid methods [Bra93], [Hac85]. Finally, the solution p^{n+1} can be inserted in (4.6-a), such that for system (4.5) we obtain the solution $(\mathbf{u}^{n+1}, p^{n+1})$ with

$$\mathbf{u}^{n+1} = \tilde{\mathbf{u}}^{n+1} - \delta t \nabla p^{n+1}.$$

Since the projection method of Chorin is only first order accurate, [Pro97, Chap. 6], projection schemes of higher order were developed. Van Kahn proposed a method that combines the advantages of the projection idea with a discretization approach of second order (Crank-Nicolson). In this formulation the Poisson equation is solved for the pressure correction $\pi^{n+1} := p^{n+1} - p^n$. For details of van Kahn's method and a detailed discussion about projection schemes we refer to [Pro97].

Combining the operator splitting method and the projection method of Chorin, the Navier Stokes equations (4.1) is split as follows

$$\frac{\tilde{\mathbf{u}}^{n+1} - \mathbf{u}^n}{\delta t} = -\operatorname{div}(\mathbf{u}^n \otimes \mathbf{u}^n) + \mathbf{f} \tag{4.8-a}$$

$$\frac{\mathbf{u}^{n+1} - \tilde{\mathbf{u}}^{n+1}}{\delta t} = \frac{1}{\rho} \operatorname{div} \mathbf{S}(\mathbf{u}^n) \tag{4.8-b}$$

$$\Delta p^{n+1} = \frac{\operatorname{div} \tilde{\mathbf{u}}^{n+1}}{\rho \, \delta t} \tag{4.8-c}$$

$$\mathbf{u}^{n+1} = \tilde{\mathbf{u}}^{n+1} - \delta t \nabla p. \tag{4.8-d}$$

where $\mathbf{S}(\mathbf{u}^n) = 2\,\mu(\|\mathbf{D}(\mathbf{u}^n)\|^2)\mathbf{D}(\mathbf{u}^n)$ with $\mathbf{D}(\mathbf{u}^n) = \frac{1}{2}\left[\nabla \mathbf{u}^n + (\nabla \mathbf{u}^n)^T\right]$.

4.1.3 Finite Volume Method

In this section the main idea of the *finite volume method* is described [GR96], [FP02]. As starting point, the integral form of the conservation laws is used. We assume that the velocity field $\mathbf{u}$ is known. For an intensive physical quantity $\psi : J \times \mathbb{R}^n \to \mathbb{R}$ (resp. $\psi : J \times \mathbb{R}^n \to \mathbb{R}^n$) we want to solve the balance equation

$$\frac{d}{dt} \int_{\Omega} \psi \, d\mathbf{x} + \int_{\partial\Omega} \mathbf{q} \cdot \mathbf{n} \, dA = 0, \tag{4.9}$$

where $\Omega \subset \mathbb{R}^n$ with the outer normal $\mathbf{n}$ and $\mathbf{q} = \psi\mathbf{u}$ denotes the convective flux (see section 2.2). By Ω we denote the whole computational domain which is composed of N control volumes $\Omega_i \subset \mathbb{R}^n$ with cell center $\mathbf{c}_i$ for all $i = 1, \ldots, N$ (see figure 4.1). Thus, for each control volume we have to solve the local balance equation

$$\frac{\partial}{\partial t} \left(\int_{\Omega_i} \psi \, d\mathbf{x} \right) + \int_{\partial\Omega_i} \mathbf{q} \cdot \mathbf{n}_i \, dA = 0, \tag{4.10}$$

where $\mathbf{n}_i$ is the outer normal vector to Ω_i. Summing all local equations (4.10) for all control volumes results in the global conservation equation (4.9), since all surface integrals over inner control faces cancel out. The simplest method to approximate the volume integral in the balance equation (4.10) is given by

$$\psi_i(t) \cong \frac{1}{|\Omega_i|} \int_{\Omega_i} \psi(t, \mathbf{x}) \, d\mathbf{x} \tag{4.11}$$

where $|\Omega_i|$ denotes the volume of Ω_i. The value $\psi_i(t)$ of each control volume Ω_i is stored at the center point $\mathbf{c}_i$ and represents the mean value of ψ over the cell Ω_i. In the case that $\psi(t, \mathbf{x})$ is constant or linear in Ω_i, relation (4.11) is exact, otherwise $\psi_i(t)$ is an approximation of second order [FP02].

Since the second term of (4.10) is discontinuous at $\partial\Omega_i$ and represents the flux across the boundary of the cell Ω_i at time t_n, the integral is split in the sum of all edges

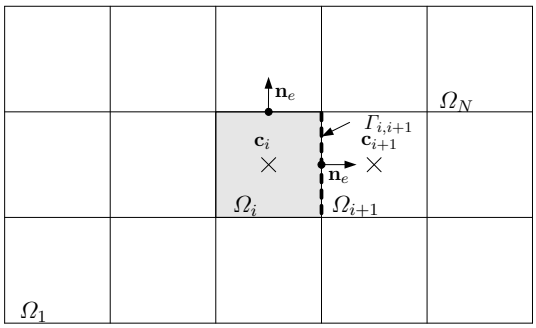


Figure 4.1: Decomposition of domain Ω in N control volumes Ω_i, $i = 1, \ldots, N$.

$e = \Gamma_{ij} := \Omega_i \cap \Omega_j$ of the cell with $\partial\Omega_i = \bigcup \Gamma_{ij}$. Thus, we obtain

$$|\Omega_i| \frac{\partial}{\partial t}\psi_i(t) + \sum_{e \subset \partial\Omega_i, e=\Gamma_{ij}} \int_{\Gamma_{ij}} \mathbf{q} \cdot \mathbf{n}_e \, dA = 0.$$

The remaining integral should be approximated using only the values $\psi_i(t)$. Therefore, it is common to introduce a function $\boldsymbol{\Psi}$, which is denoted as *numerical flux*, such that

$$\int_{\Gamma_{ij}} \mathbf{q} \cdot \mathbf{n}_e \, dA \cong |e| \, \boldsymbol{\Psi}(\psi_i, \psi_j, \mathbf{n}_e)$$

holds. If the ordinary differential system is discretized in time by the explicit Euler scheme, we obtain the formula

$$|\Omega_i| \left(\psi_i^{n+1} - \psi_i^n\right) + \delta t \left\{ \sum_{e \subset \partial\Omega_i, e=\Gamma_{ij}} |e| \, \boldsymbol{\Psi}(\psi_i, \psi_j, \mathbf{n}_e) \right\} = 0 \tag{4.12}$$

where $\psi_i^n = \psi_i(t_n)$ and ψ_i^0 is given.

In the general case, the numerical fluxes $\boldsymbol{\Psi}$ are assumed to be locally Lipschitz continuous and must satisfy the following conditions [GR96]:

$$\begin{aligned} &\text{Conservation:} && \boldsymbol{\Psi}(\psi_i, \psi_j, \mathbf{n}) = -\boldsymbol{\Psi}(\psi_j, \psi_i, -\mathbf{n}) \\ &\text{Consistency:} && \boldsymbol{\Psi}(\psi, \psi, \mathbf{n}) = \mathbf{q} \cdot \mathbf{n}. \end{aligned}$$

The conservation property means that, in the absence of source term, the approximating flux from Ω_i into Ω_j (across Γ_{ij}) is equal to the flux from of Ω_j into Ω_i.

In the following, we change the notation of space discretization, i.e., the computation domain $\Omega \subset \mathbb{R}^n$ is discretized with respect to its space dimension. In 2D, each cell is denoted by 2 different indices. Then, the field ψ is discretized in such a way that $\psi_{i,j}$ is located in the center $\mathbf{c}_{i,j}$ of cell $\Omega_{i,j}$, for all $i = 1, \ldots, N$ and $j = 1, \ldots, M$. Since the fluxes $\boldsymbol{\Psi}$ are computed over the edges, the values of $\mathbf{u} \cdot \mathbf{n}_e$ are required on the edges.

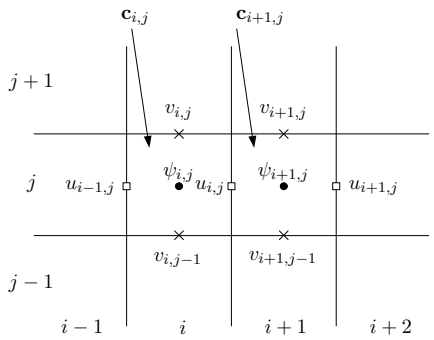


Figure 4.2: Staggered Grid.

Therefore, in the 2D case it is useful to locate the velocity components $\mathbf{u} = (u, v)$ at the center of the edges, see figure 4.2, in the 3D case they are located in the center of the faces. This type of grid is called *staggered grid*. In fact, these arrangements avoid interpolations of the velocities. Besides, the scalar pressure field is also located in the cell center $\mathbf{c}_{i,j}$, such that a strong coupling between the velocity field and the pressure is given and oscillations in the solution are avoided.

4.2 Numerical Treatment of Two-phase Flows

4.2.1 Notations for Two-phase Flows

The investigation of two-phase flow means the description of the combined behavior of two different fluids or *phases* occupying a domain $\Omega \subset \mathbb{R}^n$ that are immiscible on a molecular level, e.g., a water droplet in air. All appearing physical quantities are assumed to be continuous within each phase, but at least one physical quantity is discontinuous at the interface. Assuming that we investigate a system consisting of a liquid and a gaseous phase, we denote the domain occupied by the liquid with Ω_l and the domain occupied by the gaseous phase with Ω_g, such that $\Omega = \Omega_l \cup \Omega_g$. The two phases are separated by a sharp, smooth interface $\Gamma = \overline{\Omega}_l \cap \overline{\Omega}_g$. In general, we use the phase index l for all quantities of the liquid phase and the index g for all quantities of the gaseous phase, respectively. If the fluids are in motion, the domains $\Omega_l(t)$ and $\Omega_g(t)$ as well as the interface $\Gamma(t)$ are unknown at the time instant t. Therefore, we receive a so-called *free boundary problem*.

In general, we can distinguish three types of problems in the numerical treatment of free boundary problems [HN81].

(i) The discrete representation of the interface.

(ii) The evolution in time of the interface.

(iii) The manner in which imposed surface boundary conditions are treated.

The first two topics will be treated in section 4.2.5, whereas section 4.2.7 deals with topic three.

4.2.2 Mathematical Modeling of Surface Tension

In two-phase flows an additional force must be taken into account, in comparison to one-phase flows. Focussing on a single fluid cell $\Omega(t)$ which contains gaseous and liquid phase, the balance equation (2.15) has to be extended by surface tension forces

$$\frac{d}{dt}\int_{\Omega(t)} \rho\, \mathbf{u}\, d\mathbf{x} = \int_{\Omega(t)} \rho\, \mathbf{f}\, d\mathbf{x} + \int_{\partial\Omega(t)} \mathbf{T}(t,\mathbf{x}) \cdot \mathbf{n}\, dA + \mathbf{F}_A(t), \tag{4.13}$$

where $\Omega(t)$ is a substantial volume. The third term on the right-hand side of equation (4.13) represents the force on the intersection area $A = \Omega(t) \cap \Gamma(t)$ of the control

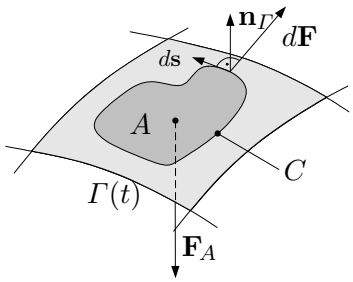


Figure 4.3: Force on a line element $d\mathbf{s}$ on the interface $\Gamma(t)$.

volume $\Omega(t)$ and the interface $\Gamma(t)$ due to surface tension (see figure 4.3). The local force $d\mathbf{F}$ acts tangential to the boundary layer $\Gamma(t)$ and perpendicular to the line element $d\mathbf{s}$ of the curve C which is the boundary of the area A. Thus, the force $d\mathbf{F}$ onto a line element $d\mathbf{s}$ is given by

$$d\mathbf{F} = \sigma \, d\mathbf{s} \times \mathbf{n}_\Gamma,$$

with the surface tension σ. Then, the imposed force $\mathbf{F}_A$ onto the area A caused by the surface tension is

$$\mathbf{F}_A(t) = \oint_C \sigma(d\mathbf{s} \times \mathbf{n}_\Gamma) = \oint_C d\mathbf{s} \times \sigma\mathbf{n}_\Gamma$$

and is directed towards the focus of the convex phase. Applying Stokes theorem leads to

$$\mathbf{F}_A(t) = \int_A (\mathbf{n}_\Gamma \times \nabla) \times \sigma\mathbf{n}_\Gamma \, dA.$$

The integrand $\mathbf{f}_\Gamma := (\mathbf{n}_\Gamma \times \nabla) \times \sigma\mathbf{n}_\Gamma$ denotes the surface tension force per unit interfacial area. It follows that

$$\begin{aligned} \mathbf{f}_\Gamma &= \nabla(\sigma\mathbf{n}_\Gamma) \cdot \mathbf{n}_\Gamma - \mathbf{n}_\Gamma(\nabla \cdot (\sigma\mathbf{n}_\Gamma)) \\ &= \nabla\sigma - \mathbf{n}_\Gamma(\mathbf{n}_\Gamma \cdot \nabla\sigma) + \sigma \underbrace{(\nabla\mathbf{n}_\Gamma) \cdot \mathbf{n}_\Gamma}_{=0} - \sigma\mathbf{n}_\Gamma(\nabla \cdot \mathbf{n}_\Gamma) \end{aligned} \tag{4.14}$$

due to $|\mathbf{n}_\Gamma|^2 = 1$. Since the term $\nabla_N \sigma := \mathbf{n}_\Gamma(\mathbf{n}_\Gamma \cdot \nabla\sigma)$ describes the gradient of σ along the normal direction to the interface, the first two terms of equation (4.14) result in the tangential part of the surface tension gradient, usually combined in[1]

$$\nabla_\Gamma \sigma := \nabla\sigma - \mathbf{n}_\Gamma(\mathbf{n}_\Gamma \cdot \nabla\sigma). \tag{4.15}$$

Thus, the surface tension density is given by

$$\mathbf{f}_\Gamma = \nabla_\Gamma \sigma - \sigma\mathbf{n}_\Gamma(\nabla \cdot \mathbf{n}_\Gamma)$$

[1]Using the projection operator $\mathbf{P} = \mathbf{I} - \mathbf{n} \otimes \mathbf{n}$ the operator ∇_Γ is given by $\nabla_\Gamma = \mathbf{P} \cdot \nabla$, since $(\mathbf{n} \otimes \mathbf{n})\mathbf{u} = (\mathbf{n} \cdot \mathbf{u})\mathbf{n}$.

where the first term describes the so-called *Marangoni forces* and the second term corresponds to the *Young-Laplace equation*. In general, the surface tension σ depends on the temperature and the concentration of surface active substances adsorbed at the interface. Taking into account that the mean curvature κ of the interface Γ is given by

$$\kappa = -\nabla \cdot \mathbf{n}_\Gamma, \tag{4.16}$$

where $\mathbf{n}_\Gamma$ is the outer normal on Γ [Ari62], the surface force results in

$$\mathbf{F}_A = \int_{\Gamma(t)} \mathbf{f}_\Gamma \, dA \qquad \text{with} \quad \mathbf{f}_\Gamma = \nabla_\Gamma \sigma + \sigma\kappa\mathbf{n}_\Gamma. \tag{4.17}$$

The momentum balance of a substantial volume $\Omega(t)$, which contains a dividing surface, is hence given by

$$\frac{d}{dt}\int_{\Omega(t)} \rho \, \mathbf{u} \, d\mathbf{x} = \int_{\Omega(t)} \rho \, \mathbf{f} \, d\mathbf{x} + \int_{\partial\Omega(t)} \mathbf{T}\cdot\mathbf{n} \, dA + \int_{\Gamma(t)} \mathbf{f}_\Gamma \, dA \tag{4.18}$$

with $\mathbf{f}_\Gamma = \nabla_\Gamma \sigma + \sigma\kappa\mathbf{n}_\Gamma$.

4.2.3 Interfacial Dirac-Distribution

In this section, we derive the divergence theorem valid for a region containing a dividing surface. For this purpose, we reproduce some important definitions and results about *distributions* [Far96], [Kan83], [Rud73]. In particular, we consider the relation between the Heaviside function to the δ-distribution.

The space $\mathcal{D}'(\mathbb{R}^n)$ denotes the dual space of $\mathcal{D}(\mathbb{R}^n) := C_0^\infty(\mathbb{R}^n)$, i.e., $\mathcal{D}'(\mathbb{R}^n)$ consists of all continuous linear functionals on the space $\mathcal{D}(\mathbb{R}^n)$ endowed with the topology that is given by the usual family of semi-norms [Yos80]. The elements of $\mathcal{D}'$ are called *generalized functions* or *distributions*. In general, we distinguish between *regular generalized functions* and *singular generalized functions*.

Definition 4.2.1 (Generalized Function) *Each continuous linear functional of $\mathcal{D}'$, which can be written in the form*

$$(f,\varphi) := \int_{\mathbb{R}} f(x)\varphi(x) \, dx, \qquad \varphi \in \mathcal{D}(\mathbb{R}),$$

with some $f \in L_{1,loc}(\mathbb{R})$ is called regular generalized function*, otherwise* singular generalized function*.*

The most famous and regarding to two-phase flows most important example for singular generalized functions is the δ-distribution.

Definition 4.2.2 (δ-Distribution) *The* δ-distribution *(resp.* Dirac-function*) is defined by the relation*

$$(\delta(x-x_0),\varphi(x)) = \varphi(x_0), \qquad \varphi \in C_0^\infty(\mathbb{R}) \text{ and } x, x_0 \in \mathbb{R}.$$

Although the δ-distribution belongs to the class of singular generalized functions*, it is often written in the symbolical notation*

$$(\delta(x-x_0),\varphi) = \varphi(x_0) =: \int_{\mathbb{R}} \delta(x-x_0)\varphi(x)\,dx, \qquad \varphi \in C_0^\infty(\mathbb{R}) \text{ and } x, x_0 \in \mathbb{R}.$$

In case that a δ-distribution appears under the integral sign, the integral stands for the functional $(\delta(x-x_0),\varphi(x))$. The derivative of a distribution is defined as follows.

Definition 4.2.3 (Generalized Derivative) *The* (generalized) derivative $D^\alpha f$ *of a generalized function $f \in \mathcal{D}'(\mathbb{R}^n)$ is defined by*

$$(D^\alpha f,\varphi) = (-1)^{|\alpha|}\,(f, D^\alpha\varphi)\,, \qquad \varphi \in \mathcal{C}_0^\infty(\mathbb{R}^n)$$

where $D = (\partial_{x_1},\ldots,\partial_{x_n})$ and $\alpha = (\alpha_1,\ldots,\alpha_n)$.

In case that $f \in C^m(\mathbb{R}^n)$, the ordinary derivative $D^\alpha f$, $|\alpha| \le m$, and the generalized derivative are identical, whereas in case that f is a discontinuous function both derivatives are different. If there is such an ambiguity in the interpretation of the derivatives, a tilde over the differential symbol designates the generalized derivative, i.e., we write $\widetilde{\partial}_x f(x)$ in one dimension and $\widetilde{D}^\alpha f(\mathbf{x})$ resp. $\widetilde{\nabla} f(\mathbf{x})$ in several-dimensions.

First, we introduce the one-dimensional Heaviside function which is defined by

$$H(x) = \begin{cases} 1 & \text{for } x \ge 0, \\ 0 & \text{for } x < 0 \end{cases}$$

and is related to the δ-distribution [Con74]. The relation between the Heaviside function H and the δ-distribution can be seen from the definition of the generalized derivative. Let $\varphi \in \mathcal{D}(\mathbb{R})$, then we get

$$(\partial_x H(x),\varphi(x)) = (H(x), -\partial_x\varphi(x)) = -\int_0^\infty \partial_x\varphi(x)\,dx = \varphi(0).$$

Thus, we obtain that in one spatial dimension the δ-distribution is the generalized derivative of the local integrable one-dimensional Heaviside function

$$\widetilde{\partial}_x H(x) = \delta(x). \tag{4.19}$$

Next, we consider a piecewise smooth function $f : [a,b] \to \mathbb{R}$ with one discontinuity at $x_0 \in [a,b]$ and a jump at this point defined by the relation

$$[f] := \lim_{h\to 0+} \left(f(x_0+h) - f(x_0-h)\right). \tag{4.20}$$

Let $\varphi \in \mathcal{D}(\mathbb{R})$ with $\operatorname{supp}\varphi = [a,b]$. Then, the generalized derivative of $f(x)$ is given by

$$\begin{aligned}(\partial_x f(x),\varphi(x)) &= -\left(f(x),\partial_x\varphi(x)\right) \\ &= -\left(\int_a^{x_0} f(x)\partial_x\varphi(x)\,dx + \int_{x_0}^b f(x)\partial_x\varphi(x)\,dx\right) \\ &= \int_{[a,b]\setminus\{x_0\}} \partial_x f(x)\varphi(x)\,dx + (f(x_0+) - f(x_0-))\varphi(x_0) \end{aligned} \tag{4.21}$$

By means of equation (4.20) and definition 4.2.2 of the δ-distribution, we write equation (4.21) symbolically as

$$\widetilde{\partial}_x f(x) = \partial_x f_c(x) + [f]\ \delta(x - x_0),$$

where we subscript the function f with the index c, which means that the jump is no longer contained in f, i.e., f_c is given by

$$f_c(x) := f(x) - [f]\ H(x - x_0).$$

The original discontinuous function f can be recovered by symbolically integration of $\widetilde{\partial}_x f$, i.e., we get

$$f(x) = \int_{[a,x]\setminus\{x_0\}} \partial_x f_c(x)\ dx + f(a) + [f]\ H(x - x_0) \quad \text{for } a < x_o < x.$$

In two-phase flows several quantities appear which are discontinuous precisely at the interface Γ, e.g., density and viscosity. The interface Γ can be a single continuous surface or group of closed surfaces and can be defined by a smooth function $\phi : \mathbb{R}^n \to \mathbb{R}$ with $\nabla\phi \neq 0$, which represents the interface by means of

$$\Gamma = \{\mathbf{x} \in \mathbb{R}^n |\ \phi(\mathbf{x}) = 0\}\,. \tag{4.22}$$

Since the gradient of the function ϕ is perpendicular to the surfaces of ϕ and points in the direction of increasing ϕ, for each point $\mathbf{x}_\Gamma$ of the interface the local unit normal in $\mathbf{x}_\Gamma$ is given as

$$\mathbf{n}_\Gamma = \frac{\nabla\phi}{|\nabla\phi|}. \tag{4.23}$$

Let Ψ be a scalar or vector field $\Psi : \mathbb{R}^n \to \mathbb{R}$ resp. $\Psi : \mathbb{R}^n \to \mathbb{R}^n$. Then, the jump across this interface is defined as

$$[\Psi](\mathbf{x}) := \lim_{h \to 0+} \left(\Psi(\mathbf{x} + h\mathbf{n}_\Gamma) - \Psi(\mathbf{x} - h\mathbf{n}_\Gamma)\right), \tag{4.24}$$

where $\mathbf{n}_\Gamma$ is the normal vector on Γ.

Then, the distribution $\delta(\phi)$ according to Gel'fand and Shilov [GS64] is defined as follows. We follow the representation of Kanwal [Kan83, Chapter 5]. Let ξ_1, ξ_2, ξ_3 be a coordinate system with $\xi_1 = \phi$ and let $\varphi(\mathbf{x}) \in C_0^\infty(\mathbb{R}^3)$. By the transformation theorem, we obtain

$$\begin{aligned}
(\delta(\phi), \varphi) &= \int \delta(\phi)\varphi(\mathbf{x})\ d\mathbf{x} \\
&= \int \delta(\xi_1)\psi(\xi_1, \xi_2, \xi_3)\ J\ d\xi_1\ d\xi_2\ d\xi_3 \\
&= \int_{\xi_1 = 0} \psi(0, \xi_2, \xi_3)\ J(0, \xi_2, \xi_3)\ d\xi_2\ d\xi_3
\end{aligned} \tag{4.25}$$

where $\psi(\xi_1, \xi_2, \xi_3) = \varphi(x_1, x_2, x_3)$ and J is the Jacobian determinant. The result that the value of the integral in (4.25) is independent of the coordinate system and defines a distribution concentrated on Γ is proven by Gel'fand and Shilov.

$$(\delta(\phi), \varphi) = \int_\Gamma \varphi(\mathbf{y})\, dA(\mathbf{y})\, \frac{1}{|\nabla\phi|}. \tag{4.26}$$

Thus, a volume integral can be transformed via the δ-distribution into a surface integral.

Then, the generalized divergence of a vector field Ψ is given by

$$\widetilde{\nabla} \cdot \Psi = \nabla \cdot \Psi_c + [\Psi] \cdot \nabla\phi\, \delta(\phi) \tag{4.27}$$

and the generalized gradient of a scalar field Ψ is given by

$$\widetilde{\nabla}\Psi = \nabla\Psi_c + [\Psi]\nabla\phi\, \delta(\phi). \tag{4.28}$$

For a proof of (4.27) and (4.28) we refer to [Kan83].

Finally, we formulate the divergence theorem for a region containing a dividing surface. Farassat [Far96] shows that the theorem remains valid for discontinuous vector fields, if all arising derivatives are replaced by generalized derivatives. Thus, the divergence theorem is valid in the following form

$$\int_\Omega \widetilde{\nabla} \cdot \Psi\, d\mathbf{x} = \int_{\partial\Omega} \Psi \cdot \mathbf{n}\, dA.$$

Thereby, we can formulate the divergence theorem for a region containing a dividing surface by means of equations (4.27) and (4.26).

Theorem 4.2.1 (Divergence Theorem) *Let $\Omega \subset \mathbb{R}^n$ be a domain, which contains a surface Γ, represented by equation (4.22). Further, let Ψ be a vector field $\Psi : \Omega \to \mathbb{R}^n$, where the only discontinuities of Ψ comes from the jump at the interface Γ. Then*

$$\int_{\Omega\setminus\Gamma} \nabla \cdot \Psi_c\, d\mathbf{x} = \int_{\partial\Omega} \Psi \cdot \mathbf{n}\, dA - \int_\Gamma [\Psi] \cdot \mathbf{n}_\Gamma\, dA,$$

where the jump $[\Psi]$ is defined by equation (4.24), $\mathbf{n}$ denotes the outwards normal vector on $\partial\Omega$, and $\mathbf{n}_\Gamma$ is the normal vector on the interface Γ.

4.2.4 Interfacial Jump Conditions

The integral balance equations for momentum and mass derived in chapter 2 are valid in the whole domain Ω, i.e., also across the interface Γ, whereas the differential equations are only valid in the interior of each phase Ω_g (resp. Ω_l). Therefore, additional conditions at the interface are required. This conditions are called *interfacial jump conditions*.

In order to derive the jump conditions, we refer to [Del74], [Sla99] and[Whi92]. We cut out a substantial ball $B_r := B_r(\mathbf{x}_\Gamma)$ with radius r and center $\mathbf{x}_\Gamma \in \Gamma(t)$ of the two-phase flow as depicted in figure 4.4. Let $\Gamma_r(t) := B_r \cap \Gamma(t)$. Thus, the ball B_r is composed

by $B_r = B_g(t) \cup B_l(t) \cup \Gamma_r(t)$ where $B_g(t)$ and $B_l(t)$ are geometrical volumes, i.e., the volumes can move with an arbitrary velocity whereas B_r moves with the particle velocity. Since the volume B_r is substantial, the surfaces $\partial B_g \backslash \Gamma$ and $\partial B_l \backslash \Gamma$ are also substantial, whereas the interface $\Gamma(t)$ is non-substantial. Hence, the velocity of the interface has not be identical to the particle velocity and phase change processes are permitted. Therefore, for each point belonging to the boundary $S := \partial B_g \backslash \Gamma$ (resp. $S := \partial B_l \backslash \Gamma$) holds

$$\mathbf{u}_g \cdot \mathbf{n} = \mathbf{u}_S \cdot \mathbf{n} \quad (\text{resp.} \quad \mathbf{u}_l \cdot \mathbf{n} = \mathbf{u}_S \cdot \mathbf{n}), \tag{4.29}$$

where $\mathbf{u}_S$ is the velocity of the displacement of the surface S, $\mathbf{u}_g$ (resp. $\mathbf{u}_l$) the velocity of the particle, and $\mathbf{n}$ the outer normal to ∂B_r.

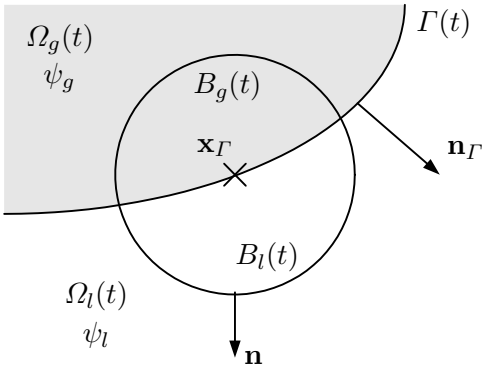


Figure 4.4: Illustration of the domain decomposition for the derivation of the jump conditions.

For an intensive physical quantity ψ, which is discontinuous at the interface and acts inside the substantial ball B_r, holds

$$\frac{d}{dt}\int_{B_r} \psi \, d\mathbf{x} = \frac{d}{dt}\int_{B_g(t)} \psi_g \, d\mathbf{x} + \frac{d}{dt}\int_{B_l(t)} \psi_l \, d\mathbf{x} + \frac{d}{dt}\int_{\Gamma_r(t)} \psi_\Gamma \, dA, \tag{4.30}$$

where ψ_Γ is only defined on the surface $\Gamma(t)$.

On the assumption that the interface Γ is thin and massless (jump conditions for interfaces of finite thickness can be found in [Ish75], [Gat96]), the third integral on the right-hand side of equation (4.30) vanishes for $\psi = \rho$. In this case the momentum $\psi = \rho\mathbf{u}$ of the interface can also be neglected [Ish75], such that we omit the third integral term in the following provided that ψ is given as desired.

The normal vectors at the interface $\Gamma_r(t)$ are related by $\mathbf{n}_\Gamma = \mathbf{n}_g = -\mathbf{n}_l$. Since $B_g(t)$ and $B_l(t)$ are non-substantial volumes, we apply the Leibniz rule 2.2.2 to equation (4.30),

using equation (4.29), and obtain

$$\begin{aligned}\frac{d}{dt}\int_{B_r}\psi\,d\mathbf{x} &= \int_{B_g(t)}\frac{\partial}{\partial t}\psi_g\,d\mathbf{x}+\int_{\partial B_g(t)\setminus\Gamma_r(t)}\psi_g\mathbf{u}_g\cdot\mathbf{n}\,dA+\int_{\Gamma_r(t)}\psi_g\mathbf{u}_\Gamma\cdot\mathbf{n}_\Gamma\,dA\\ &\quad+\int_{B_l(t)}\frac{\partial}{\partial t}\psi_l\,d\mathbf{x}+\int_{\partial B_l(t)\setminus\Gamma_r(t)}\psi_l\mathbf{u}_l\cdot\mathbf{n}\,dA+\int_{\Gamma_r(t)}\psi_l\mathbf{u}_\Gamma\cdot(-\mathbf{n}_\Gamma)\,dA\\ &= \int_{B_r(t)\setminus\Gamma_r(t)}\frac{\partial}{\partial t}\psi\,d\mathbf{x}+\int_{\partial B_r(t)}\psi\mathbf{u}\cdot\mathbf{n}\,dA-\int_{\Gamma_r(t)}[\psi]\mathbf{u}_\Gamma\cdot\mathbf{n}_\Gamma\,dA \qquad (4.31)\end{aligned}$$

where the jump $[\psi]$ is given by equation (4.24), i.e., in this case we get $[\psi]=\psi_l-\psi_g$. The application of the divergence theorem 4.2.1 to equation (4.31) yields

$$\begin{aligned}\frac{d}{dt}\int_{B_r}\psi\,d\mathbf{x}=\int_{B_r(t)\setminus\Gamma_r(t)}\frac{\partial}{\partial t}\psi\,d\mathbf{x}+\int_{B_r(t)\setminus\Gamma_r(t)}\nabla\cdot\psi\mathbf{u}\,d\mathbf{x}\\ +\int_{\Gamma_r(t)}[\psi\,(\mathbf{u}-\mathbf{u}_\Gamma)]\cdot\mathbf{n}_\Gamma\,dA.\end{aligned}$$

We summarize this result in the transport theorem valid for a region containing a dividing surface [Sla99].

Theorem 4.2.2 (Transport Theorem for 2 Phase-Flows) *Let $\mathbf{u}\in C^1(J\times\Omega;\mathbb{R}^n)$ be bounded. For each $(t_0,\mathbf{x}_0)\in J\times\Omega$ is $\Phi(t;t_0,\mathbf{x}_0)$ solution of*

$$\frac{\partial}{\partial t}\Phi(t)=\mathbf{u}(t,\Phi(t)),\qquad \Phi(t_0)=\mathbf{x}_0.$$

For $B_0\subset\Omega$ compact and $\partial B_0\in C^1$ let

$$B(t)=\{\Phi(t;t_0,\mathbf{x}_0):\mathbf{x}_0\in B_0\}$$

be the volume moving with the velocity $\mathbf{u}$. Furthermore, $B(t)$ contains a dividing surface $\Gamma(t)$ and let ψ be a scalar or vector field, where the only jump of ψ comes from the discontinuity on the interface $\Gamma(t)$. Then

$$\frac{d}{dt}\int_{B(t)}\psi\;\;d\mathbf{x}\;=\;\int_{B(t)\setminus\Gamma(t)}\left(\frac{\partial}{\partial t}\psi+\operatorname{div}(\psi\mathbf{u})\right)\;\;d\mathbf{x}\;+\;\int_{\Gamma(t)}[\psi\,(\mathbf{u}-\mathbf{u}_\Gamma)]\;\cdot\;\mathbf{n}_\Gamma\;\;dA,$$

where $\mathbf{u}_\Gamma$ is the velocity of the interface Γ, $\mathbf{n}_\Gamma$ its normal vector, and the jump of ψ is given by equation (4.24).

For the mass balance equation, we deduce from the transport theorem 4.2.2 with $\psi=\rho$ the differential equation with its corresponding jump condition on $B_r(t)$. On the assumption that the interface is thin and massless, the third integral on the right-hand side of equation (4.30) vanishes for $\psi=\rho$. Division by $|B_r(t)|$ and $r\to 0+$ results in

$$\begin{aligned}\frac{\partial}{\partial t}\rho+\operatorname{div}(\rho\mathbf{u}) &= 0 \text{ in } \Omega_g\cup\Omega_l &(4.32\text{-a})\\ [\rho\,(\mathbf{u}-\mathbf{u}_\Gamma)]\cdot\mathbf{n}_\Gamma &= 0 \text{ on } \Gamma. &(4.32\text{-b})\end{aligned}$$

We turn to the momentum balance equation (4.18), apply the transport theorem 4.2.2 with $\psi = \rho\mathbf{u}$ and use for the integral containing the stress tensor $\mathbf{T}$ the divergence theorem 4.2.1. This yields

$$\begin{aligned}\int_{B_r(t)\setminus\Gamma_r(t)} \left(\frac{\partial}{\partial t}(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u})\right)\, d\mathbf{x} = &-\int_{\Gamma_r(t)} [\rho\mathbf{u}\otimes(\mathbf{u}-\mathbf{u}_\Gamma)]\cdot\mathbf{n}_\Gamma\, dA \\ &+\int_{B_r(t)\setminus\Gamma_r(t)} \mathbf{f}\rho\, d\mathbf{x} + \int_{B_r(t)\setminus\Gamma_r(t)} \nabla\cdot\mathbf{T}\, d\mathbf{x} \\ &+\int_{\Gamma_r(t)} [\mathbf{T}]\cdot\mathbf{n}_\Gamma\, dA + \int_{\Gamma_r(t)} (\sigma\kappa\mathbf{n}_\Gamma + \nabla_\Gamma\sigma)\, dA.\end{aligned}$$

Division by $|B_r(t)|$ and $r\to 0+$ results in

$$\begin{aligned}\frac{\partial}{\partial t}(\rho\mathbf{u}) + \operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u}) &= \operatorname{div}\mathbf{T} + \mathbf{f} && \text{in } \Omega_g\cup\Omega_l && \text{(4.33-a)}\\ [\rho\mathbf{u}\otimes(\mathbf{u}-\mathbf{u}_\Gamma) - \mathbf{T}]\cdot\mathbf{n}_\Gamma &= \sigma\kappa\mathbf{n}_\Gamma + \nabla_\Gamma\sigma && \text{on } \Gamma, && \text{(4.33-b)}\end{aligned}$$

the differential equation with its corresponding jump condition.

For the subsequent part we state the following assumptions.

Assumption 4.2.1 *We assume that*

(i) the fluid is incompressible.

(ii) there is no phase change process.

(iii) the surface tension is constant.

(iv) there are no-slip conditions at the interface.

From assumption 4.2.1 we infer the following simplifications for the interfacial jump conditions. Jump condition (4.32-b) leads to the equality of the one-sided limits of the interfacial mass flux $\dot{m}$, i.e.,

$$\rho_g(\mathbf{u}_g - \mathbf{u}_\Gamma)\cdot\mathbf{n}_\Gamma = \rho_l(\mathbf{u}_l - \mathbf{u}_\Gamma)\cdot\mathbf{n}_\Gamma =: \dot{m}.$$

The exclusion of phase change processes means that no source terms concerning mass act on the interface. Hence, the interfacial mass flux vanishes, i.e., $\dot{m} = 0$. As a result we get that the normal component of the gaseous phase towards the interface $\mathbf{u}_g\cdot\mathbf{n}_\Gamma$ equals the normal velocity of the interface displacement $\mathbf{u}_\Gamma\cdot\mathbf{n}_\Gamma$. In addition, the same relation is valid for the liquid phase. Therefore, we obtain

$$\mathbf{u}_g\cdot\mathbf{n}_\Gamma = \mathbf{u}_\Gamma\cdot\mathbf{n}_\Gamma = \mathbf{u}_l\cdot\mathbf{n}_\Gamma.$$

Combining these relations, we obtain the jump condition for the normal component of the velocity

$$[\mathbf{u}]\cdot\mathbf{n}_\Gamma = 0. \tag{4.34}$$

In fact, the conditions at the interface are incomplete, since there is no information about the tangential components. For viscous fluids it is common to assume no-slip conditions at the interface, i.e.,

$$[\mathbf{u}] \cdot \mathbf{t}_\Gamma = 0, \tag{4.35}$$

where $\mathbf{t}_\Gamma$ is any tangential vector to the interface. Combining relation (4.34) and (4.35) results in

$$[\mathbf{u}] = 0.$$

In other words, the velocity is continuous at the interface.

The requirement that the surface tension is constant results in $\nabla_\Gamma \sigma = 0$. Therefore, the first term in equation (4.17) of the surface tension density $\mathbf{f}_\Gamma$ vanishes and

$$\mathbf{f}_\Gamma = \sigma\kappa\mathbf{n}_\Gamma$$

remains. Hence, the Marangoni forces are neglected. Turning to the jump condition of the momentum balance equation (4.33) and using additionally the continuity of the velocity at the interface, we obtain

$$-[\mathbf{T}] \cdot \mathbf{n}_\Gamma = [p\mathbf{I} - \mathbf{S}] \cdot \mathbf{n}_\Gamma = \sigma\kappa\mathbf{n}_\Gamma,$$

where equation (2.25) is used for the total stress tensor $\mathbf{T}$. Since the interfacial jump in the pressure p is usually dominates, it is useful to split the jump condition in two separated terms:

$$[p] \cdot \mathbf{n}_\Gamma + \mathbf{n}_\Gamma \cdot [-\mathbf{S}] \cdot \mathbf{n}_\Gamma = \sigma\kappa \quad \text{and} \quad \mathbf{t}_\Gamma \cdot [-\mathbf{S}] \cdot \mathbf{n}_\Gamma = 0,$$

i.e., the tangential components of the stress tensor at the interface are continuous. Then, the condition concerning the stress tensor has to be taken into account by the interpolation of the viscosities [TBET98].

In summary, the differential equations for momentum and mass with corresponding jump conditions read as

$$\begin{array}{lrcll}
\text{Momentum balance:} & \frac{\partial}{\partial t}\rho\mathbf{u} + \operatorname{div}(\rho\mathbf{u} \otimes \mathbf{u}) & = & \operatorname{div}\mathbf{T} + \mathbf{f} & \text{in } \Omega_g \cup \Omega_l \\
& [p\mathbf{I} - \mathbf{S}] \cdot \mathbf{n}_\Gamma & = & \sigma\kappa\mathbf{n}_\Gamma & \text{on } \Gamma \\
\text{Mass balance:} & \operatorname{div}\mathbf{u} & = & 0 & \text{in } \Omega_g \cup \Omega_l \\
& [\mathbf{u}] & = & 0 & \text{on } \Gamma \\
\text{Normal velocity of } \Gamma\text{:} & V & = & \mathbf{u} \cdot \mathbf{n} & \text{on } \Gamma.
\end{array} \tag{4.36}$$

4.2.5 Numerical Treatment of the Interface

For the numerical description of free boundary problems, different methods were developed to treat the interface. In principal, the methods can be divided into two classes: the so-called *front tracking* methods and *front capturing* methods.

The front tracking method bases on a Lagrangian formulation where the interface is represented by a separate unstructured grid (surface grid) the nodes of which are convected with a local velocity; details can be found in [UT92], [ET98], [ET99]. The advantage of front tracking methods is that the interface is exactly determined by the position of the surface grid such that interfacial conditions can be incorporated rather easily. In addition, the curvature can be approximated well such that surface tension can be taken into account. A disadvantage of this method is that flows with strong interface deformations such as bubble break-up and coalescence can only be computed using additional algorithms, since the surface grid will then be strongly distorted.

In contrast, the front capturing method is an Eulerian formulation of the interface evolution where the interface is captured by a scalar function on a stationary grid. The first methods in this area have been the *marker-and-cell (MAC) method* [HW65] where *marker particles* are convected for each fluid, and the *volume-of-fluid (VOF) method* [HN81] where a *marker function* is convected. Phenomena as bubble break-up and coalescence can be computed directly, since the interface is implicitly captured in front capturing methods. The two main difficulties in the use of front capturing methods are the maintenance of a sharp boundary between the different fluids and the accurate computation of the surface tension forces [TBET98]. The first issue led to the development of different methods, e.g., to the *level set (LS) method*. Both issues will be discussed in the following and the LS and VOF methods are introduced.

For another method which can be described as a hybrid between a front capturing and a front tracking method, we refer to Tryggvason et al. [TBET98], where also a survey about different methods is given. Another approach, which is also based on Eulerian and Lagrangian methods, was developed for flows over a complex geometry, the so-called *immersed-boundary (IB) method* [Pes82], [Pes02]. In contrast to unstructured grid methods an obstacle in a flow field is considered to be a kind of momentum force rather than a real body [KKC01]. The main drawback of this method is also that for the simulation of bubble break-up and coalescence special algorithms have to be developed. A comparison of the VOF and IB method is given in [LF04]. In [RK95], Rider and Kothe compare interface tracking methods, among others the LS and VOF method.

Since we are interested in the description of strongly deformed bubbles or droplets, we concentrate on front capturing methods, especially on the LS and the VOF method.

The Level Set Method

Let $\phi : J \times \Omega \to \mathbb{R}$ be a continuous function which implicitly represents the interface Γ by

$$\phi(t, \mathbf{x}) = 0. \tag{4.37}$$

The regions of the phases are then defined by the relations

$$\begin{cases} \phi(t, \mathbf{x}) > 0 & \text{for } \mathbf{x} \in \Omega_l, \\ \phi(t, \mathbf{x}) < 0 & \text{for } \mathbf{x} \in \Omega_g. \end{cases} \tag{4.38}$$

For the evolution of the implicit function ϕ, the transport equation

$$\frac{\partial}{\partial t}\phi + \mathbf{u} \cdot \nabla\phi = 0 \tag{4.39}$$

is employed. Equation (4.39) is sometimes denoted as *level set equation* and describes the motion of the interface where $\phi(t, \mathbf{x}) = 0$. Equations (4.37)-(4.39) describe the so-called *LS method*. A typical choice for ϕ is that of a *signed distance function*. The normal vector $\mathbf{n}_\Gamma$ on the interface Γ can be computed using equation (4.23). Other methods were developed as the so-called *fast marching method* based on the assumption that the investigated flow only expands in one direction, which was introduced by Sethian. For more details on the LS method and variations for special flow types we refer to [OF03].

The Volume of Fluid Method

The VOF method was first introduced by Hirt and Nicols [HN81] and is based on the concept of the fractional volume of fluid. The marker function corresponds to the fractional volume of the cell occupied by fluid and can be understood as the discretized version of the characteristic function f of the liquid phase, i.e., $f = 1$ inside Ω_l, $f = 0$ inside Ω_g.

Then, the value of $f = 1$ indicates a cell full of liquid, while a zero value marks a cell which contains no liquid. Cells with f value between zero and one must then contain a free surface (see figure 4.5).

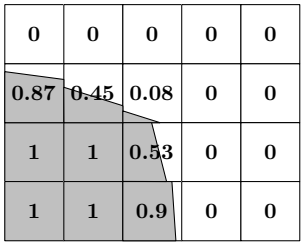


Figure 4.5: Illustration of the VOF-variable f.

Definition 4.2.4 (VOF-Function/ VOF-Variable) *The characteristic function f, used for the flow description, is called* VOF-function*, or* VOF-variable*.*

The evolution of the VOF-variable f is given by the transport equation

$$\frac{\partial}{\partial t}f + \mathbf{u} \cdot \nabla f = 0. \tag{4.40}$$

In contrast to the function ϕ of the LS method, the VOF-function f is discontinuous on the continuous level and has extremely steep gradients at the interface on the discretized level. Therefore, an algorithm has been devised for accurately computing the evolution of f. The fact that f is a step function with values of zero or one permits the usage of a flux approximation that preserves its discontinuous nature, known as donor-acceptor

method [HN81]. Finally, if in an interface cell the normal vector at the interface and the value of f (i.e., the volume fraction) are known, a plane which approximates the interface can be constructed. Before we deal with these aspects in more detail, we turn to the computation of the interface normal vector using the derivatives of f.

Considering a two-phase flow, the characteristic function f is given by

$$f(t, \mathbf{x}) = H(\phi(t, \mathbf{x}))$$

where $H(\phi)$ is the Heaviside function and ϕ is defined by equations (4.37) and (4.38). Using relation (4.19) combined with the chain rule or applying equation (4.28), we obtain

$$\widetilde{\nabla} f = \widetilde{\nabla} H(\phi) = \delta(\phi) \nabla \phi \tag{4.41}$$

for the generalized derivative of the characteristic function $\widetilde{\nabla} f$ and, formally,

$$\left| \widetilde{\nabla} f(t, \mathbf{x}) \right| = \delta(\phi) |\nabla \phi| \tag{4.42}$$

for its absolute value. In section 4.2.6 we consider $|\nabla f|$ using geometric measure theory and thereby obtain an explicit representation of $|\nabla f|$. Combining (4.41),(4.42) and (4.23) results in the following representation for the unit normal vector at the interface Γ

$$\mathbf{n}_\Gamma = \frac{\widetilde{\nabla} f}{\left| \widetilde{\nabla} f \right|}. \tag{4.43}$$

As mentioned at the beginning of this section, the accurate computation of the surface tension plays a decisive role. In order to recognize this, we combine the equation for the curvature (4.16) with the equation of the unit normal vector (4.43) and get

$$\kappa = -\nabla \cdot \left(\frac{\widetilde{\nabla} f}{\left| \widetilde{\nabla} f \right|} \right).$$

Thus, the curvature is obtained as the second derivative of a discontinuous function which is a numerical challenge (see section 4.2.7).

For the accurate solution of the evolution equation (4.40) for f, a special algorithm has been devised, since a standard finite-difference approximation would lead to a smearing of function f (numerical diffusion), i.e., information for the definition of the interface is lost. On the other hand, numerical methods of higher order lead to oscillation of f near the interface.

In order to avoid these undesirable effects, the transportation of f is computed in such a way that its discontinuous nature can be preserved. Therefore, the fact that f is a characteristic function can be used. The important point is that the fluxes across the grid cell faces are computed accurately. In order to achieve this, it is advantageous to know the position of the interface, i.e., to reconstruct the interface. The first approach

of interface reconstruction, goes back on Noh and Woodward [NW76] and is known as *simple line interface calculation (SLIC)*, wherein the interfaces are described by planes which are parallel to the grid cell faces. An advanced method reconstructs the interface as planes that truncate cells with a volume equal to to the fluid volume in that cell. This approach is known as *piecewise linear interface calculation (PLIC)* [You82], [SZ99]. A detailed description of reconstruction is given by Rider and Kothe [RK98]. In figure 4.5, the PLIC approach is depicted.

Further improvements of the VOF method and the reconstruction were developed by [LNS+94], [Rud97]. For the reconstruction on unstructured grids we refer to [GW01].

Comparison of the VOF Method and LS Method

A common property of the VOF and LS method is that only one additional scalar field is required, independent of the number of discontinuous quantities, e.g., for density and viscosity. The LS method has the particular advantage that the interface is representable as a continuous surface and no subsequent reconstruction is necessary. On the other hand, one disadvantage of the LS method is that the function ϕ has to be re-initialized in each time-step which leads to problems concerning mass conservation. Thus, the main significant distinction between these methods is that in case of the LS method the mass is not exactly conserved in contrast to the VOF method. In fact, the mass of the dispersed phase decreases significantly in the simulation, e.g., see [RK95], [SP00]. One possibility to reduce this decrease is given by Sussman and Puckett [SP00], wherein they suggested a combination of the VOF and LS method. Additionally, this approach can be used to reduce parasitic currents (see subsection 4.2.7).

4.2.6 Interfacial Area

The VOF function f plays a decisive role in the considerations of two-phase flow problems. Equation (4.19) shows that the derivative of the Heaviside function is related to the δ-distribution, respectively, equation (4.41) shows that ∇f is related to the δ-distribution. We saw that the δ-distribution can be used to transform a surface integral into a volume integral and we received a formal representation for $|\nabla f|$ (see equation (4.42)). In this section we show that $|\nabla f|$ is not a distribution and can be represented in an explicit form of the interfacial area. For this purpose we show that $|\nabla f|$ can be used to compute the interfacial area of $\Gamma = \{\mathbf{x} \in \Omega |\ \phi(\mathbf{x}) = 0\}$, i.e.,

$$\text{Interfacial Area inside } \Omega = \int_{\Omega} |\nabla f|\ d\mathbf{x}. \tag{4.44}$$

In order to show this, we introduce some generalizations and reproduce some definitions and results from geometric measure theory. In the following, we omit the "tilde" symbol for the generalized derivatives.

We consider the characteristic function χ_E

$$\chi_E(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{x} \in E \\ 0 & \text{if } \mathbf{x} \notin E, \end{cases}$$

which corresponds to the subset $E \subset \mathbb{R}^n$ and denote by $D\chi_E$ its generalized derivative. If the set E is bounded, the *n-dimensional Lebesgue measure of* $E \cap \Omega$, denoted with $\mathcal{L}^n(E)$, is given by

$$\mathcal{L}^n(E) := \int_\Omega \chi_E \, d\mathbf{x}$$

and $\chi_E \in L_1(\Omega)$, but $\chi_E \notin W_1^1(\Omega)$. We are interested in the measure of the boundary set $|\partial E \cap \Omega|$, but the boundary set $|\partial E \cap \Omega|$ has Lebesgue measure zero.

In order to measure subsets of $\mathbb{R}^n$ of lower dimension, we introduce the *Hausdorff measure* $\mathcal{H}^s$, defined in terms of the diameters of various coverings [EG92].

Definition 4.2.5 (Hausdorff measure) *Suppose $A \subset \mathbb{R}^n$, $0 < \delta \leq \infty$, and let s be a nonnegative integer. We define*

$$\mathcal{H}^s_\delta(A) := \inf \left\{ 2^{-s}\alpha_s \sum_{j=1}^{\infty} (\text{diam } A_j)^s \;\middle|\; A \subset \sum_{j=1}^{\infty} A_j, \text{ diam } A_j < \delta \right\}$$

where $\alpha_s = \mathcal{L}^s(B_1(0))$. Then, the s-dimensional Hausdorff measure *is defined by*

$$\mathcal{H}^s(A) := \lim_{\delta \to 0+} \mathcal{H}^s_\delta(A) = \sup_{\delta > 0} \mathcal{H}^s_\delta(A).$$

The requirement $\delta \to 0+$ ensures that the coverings are conformed to the local geometry of the set A. The s-dimensional Hausdorff measure can be extended to real dimensions, by replacing α_s by the corresponding expressions in terms of gamma functions ($\alpha_s = \Gamma(1/2)^s / \Gamma(s/2+1)$) [Giu84], [MR01]. For $\delta > \rho$ it follows from the definition that $\mathcal{H}^s_\rho \geq \mathcal{H}^s_\delta$, and in particular $\mathcal{H}^s_\infty(A) = 0$ holds if and only if $\mathcal{H}^s(A) = 0$ [Giu84].

The n-dimensional Lebesgue measure and the n-dimensional Hausdorff measure are related to each other,

$$\alpha_n \mathcal{H}^n(E) = \mathcal{L}^n(E),$$

with $\alpha_n := \mathcal{L}^s(B_1(0))$. Furthermore, we point out that the Hausdorff measure $\mathcal{H}^0$ is just the counting measure, and $\mathcal{H}^1$ corresponds to the line integral. We assume that $\mathbf{f} : \mathbb{R} \to \mathbb{R}^n$, $n \geq 1$ is Lipschitz and injective, then we define the curve $C := \mathbf{f}([a,b]) \subset \mathbb{R}^n$. From the area formula [EG92, p. 96] we infer that

$$\mathcal{H}^1(C) = \int_a^b |D\mathbf{f}(x)| \; dx$$

corresponds to the length of the curve C. As next, we assume that $M \subset \mathbb{R}^{n-1}$, $g : M \to \mathbb{R}$ and $g \in C^1(M)$. Furthermore, let G be the graph of g, i.e., $G := \left\{ (\mathbf{x}, g(\mathbf{x})) \in \mathbb{R}^n | \; \mathbf{x} \in \mathbb{R}^{n-1} \right\}$. Then,

$$\mathcal{H}^{n-1}(G) = \int_M \sqrt{1 + |\nabla g|^2} \, d\mathbf{x}$$

holds and represents the area of G by means of the coarea formula [EG92, p. 104]. Via the area and coarea formulas it can be shown that if $M \subset \mathbb{R}^n$ is an m-dimensional regular surface, $\mathcal{H}^m(M)$ is the m-dimensional area of M.

So far, the explicit representation of the hypersurface was necessary in order to determine the Hausdorff measure. In fact, the Hausdorff measure can be developed by special functions, such that the representation of the hypersurface is not needed. Therefore, we study functions on $\mathbb{R}^n$ of bounded variation, i.e., functions whose first derivatives are Radon measures [Giu84, MG03].

Definition 4.2.6 (Bounded Variation) *[Giu84] Let $\Omega \subset \mathbb{R}^n$ be an open set. A function $f \in L_1(\Omega)$ is said to have* bounded variation *in Ω if*

$$\int_\Omega |Df(x)| \; dx := \sup \left\{ \int_\Omega f \operatorname{div} g \; dx \;\middle|\; g \in C_0^1(\Omega;\mathbb{R}^n),\ |g(x)| \leq 1 \quad \forall x \in \Omega \right\} < \infty.$$

We define $BV(\Omega)$ as the space of all functions in $L_1(\Omega)$ with bounded variation.

We say that a Borel set E has *finite perimeter* if its characteristic function χ_E is of bounded variation.

In the following, we recall the Gauss-Green theorem, wherein $\partial^* E$ denotes the *reduced boundary* and is a subset of ∂E with finite perimeter. Roughly speaking, the reduced boundary contains all points $\mathbf{x} \in \partial E$ for which a measure theoretic unit normal ν_E in $\mathbf{x}$ exists, for a precise definition we refer to [Giu84, EG92]. Here, we are interested in the case that ∂E is a C^1-hypersurface and then $\partial E^* = \partial E$ holds.

Theorem 4.2.3 (Gauss-Green Theorem) *[EG92, p. 209] Let $E \subset \mathbb{R}^n$ have locally finite perimeter. For $\mathcal{H}^{n-1}$-a.e. $\mathbf{x} \in \partial^* E$, there is a unique measure theoretic unit outer normal ν_E such that*

$$\int_E \operatorname{div} g = \int_{\partial^* E} g \cdot \nu_E \; d\mathcal{H}^{n-1}$$

for all $g \in C_0^1(\mathbb{R}^n)$.

Finally, we can prove the following theorem.

Theorem 4.2.4 *Let $\Omega \subset \mathbb{R}^n$ and $E \subset \Omega$ with C^2-boundary. Then,*

$$\int_\Omega |D\chi_E| \; d\mathbf{x} = \mathcal{H}^{n-1}(\partial E \cap \Omega).$$

Proof. [Giu84]. Let $g \in C_0^1(\Omega;\mathbb{R}^n)$ and $|g(\mathbf{x})| \leq 1$. We apply theorem 4.2.3 and obtain

$$\int_\Omega \chi_E \operatorname{div} g \; d\mathbf{x} = \int_E \operatorname{div} g \; d\mathbf{x} = \int_{\partial E} g \cdot \nu_E \; d\mathcal{H}^{n-1},$$

where ν_E is the outer unit normal to ∂E. Due to $|\nu_E(\mathbf{x})| = 1$ and $|g(\mathbf{x})| \leq 1$ we obtain

$$\int_{\partial E} g \cdot \nu_E \, d\mathcal{H}^{n-1} \leq \mathcal{H}^{n-1}(\partial E \cap \Omega).$$

We infer from

$$\begin{aligned} \int_\Omega |D\chi_E(\mathbf{x})| \, d\mathbf{x} &= \sup \left\{ \int_\Omega \chi_E \operatorname{div} g \, d\mathbf{x} \;\middle|\; g \in C_0^1(\Omega;\mathbb{R}^n),\ |g(\mathbf{x})| \leq 1 \quad \forall \mathbf{x} \in \Omega \right\} \\ &\leq \mathcal{H}^{n-1}(\partial E \cap \Omega) \end{aligned}$$

that $\chi_E \in BV(\Omega)$. It remains to show that

$$\int_\Omega |D\chi_E(\mathbf{x})| \, d\mathbf{x} \geq \mathcal{H}^{n-1}(\partial E \cap \Omega)$$

holds. Since $\partial E \in C^2$, the normal vector $\nu_E \in C^1$ with $|\nu_E(\mathbf{x})| = 1$ may be extended to a function N, which is defined on $\mathbb{R}^n$, in such a way that $N \in C^1(\mathbb{R}^n;\mathbb{R}^n)$ and $|N(\mathbf{x})| \leq 1$ for all $\mathbf{x} \in \mathbb{R}^n$. Set $g := N\eta$ with $\eta \in C_0^\infty(\Omega)$ and $|\eta| \leq 1$, then we obtain

$$\int_E \operatorname{div} g \, d\mathbf{x} = \int_{\partial E} \eta N \cdot \nu_E \, d\mathcal{H}^{n-1} = \int_{\partial E} \eta \, d\mathcal{H}^{n-1}$$

by applying theorem 4.2.3 and due to $N_{|\partial E} = \nu_E$. Thus, we get

$$\begin{aligned} \int_\Omega |D\chi_E(\mathbf{x})| \, d\mathbf{x} &\geq \sup \left\{ \int_{\partial E} \eta \, d\mathcal{H}^{n-1} \;\middle|\; \eta \in C_0^\infty(\Omega),\ |\eta| \leq 1 \right\} \\ &= \mathcal{H}^{n-1}(\partial E \cap \Omega) \end{aligned}$$

□

The result of theorem 4.2.4 can be extended to sets $E \subset \Omega \subset \mathbb{R}^n$ with finite perimeter [EG92].

In summary, we deduce from theorem 4.2.4 that the VOF-function f, which corresponds to a characteristic function, can be used to determine the interfacial area inside Ω, i.e.,

$$|\Gamma| = \int_\Omega |\nabla f| \, d\mathbf{x},$$

compare equation (4.44).

4.2.7 Surface Tension

The application of front capturing methods requires special considerations in order to compute the surface tension, since the curvature κ is given by the second derivative of a discontinuous function. Different approaches were developed for an accurate computation of the surface tension.

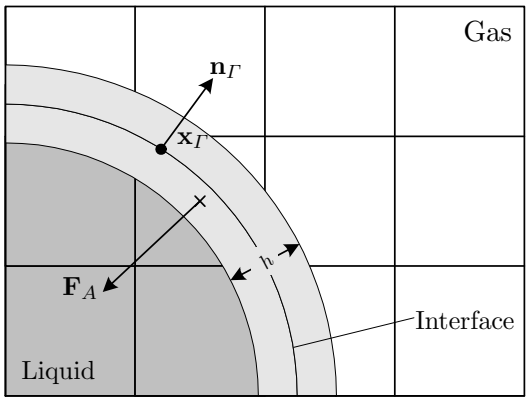


Figure 4.6: Transition zone introduced by Brackbill

The probably most famous approach is the *continuum surface force (CSF) model* of Brackbill [BKZ92], where the surface tension forces are transformed into volume forces. The interface is represented as a transition region of finite thickness h (see figure 4.6) such that the area-related surface force $\mathbf{f}_\Gamma(t, \mathbf{x}_\Gamma)$ at the interface is expressed in terms of a volume-related surface force $\mathbf{f}_{\Gamma V}(t, \mathbf{x})$ inside this transition zone. Thus, if $h \to 0$ both forces are equal, i.e.,

$$\int_{\Delta\Gamma(t)} \mathbf{f}_\Gamma(t, \mathbf{x}_\Gamma)\, dA = \lim_{h\to 0} \int_{\Delta V(t)} \mathbf{f}_{\Gamma V}(t, \mathbf{x})\, d\mathbf{x},$$

where the area $\Delta\Gamma$ lies within the small volume of integration ΔV. Additionally, Brackbills formulation requires that the volume force $\mathbf{f}_{\Gamma V}$ is equal to zero outside the transition region. Using the distance function $\phi(t, \mathbf{x}) = (\mathbf{x} - \mathbf{x}_\Gamma) \cdot \mathbf{n}_\Gamma$ with $\mathbf{n}_\Gamma = \mathbf{n}_\Gamma(\mathbf{x}_\Gamma(\mathbf{x}))$ and $\mathbf{x}_\Gamma(\mathbf{x}) = \min_{\mathbf{y}\in\Gamma} |\mathbf{x} - \mathbf{y}|$ leads to the requirement

$$\mathbf{f}_{\Gamma V} = 0 \qquad \text{for} \quad |\phi(t, \mathbf{x})| \geq h.$$

With the aid of equation (4.26) the surface force can be rewritten as a volume integral ($\phi = 0$), we obtain

$$\mathbf{F}_A(t) = \int_{\Gamma(t)} \mathbf{f}_\Gamma(t, \mathbf{x}_\Gamma)\, dA = \int_{V(t)} \mathbf{f}_\Gamma(t, \mathbf{x}) \delta\left(\phi(t, \mathbf{x})\right)\, d\mathbf{x}.$$

Thus, the volume force $\mathbf{f}_{\Gamma V}$ for finite h can be identified as $\mathbf{f}_{\Gamma V} = \mathbf{f}_\Gamma\, \delta(\phi)$. Using equation (4.17) and assuming that the surface tension is constant results in $\mathbf{f}_{\Gamma V} = \sigma\kappa\mathbf{n}_\Gamma\delta(\phi)$, combined with equation (4.43) yields

$$\mathbf{f}_{\Gamma V} = \sigma\kappa\nabla f,$$

due to $|\nabla\phi| = 1$.

Brackbill used the discontinuous *color function* $c(t, \mathbf{x})$ for the distinction of the fluids, which corresponds to the VOF-variable f_g, and replaced this color function $c(t, \mathbf{x})$ by

a smooth approximation $\tilde{c}(t, \mathbf{x})$. In case of incompressible flow problems the density function $\rho(t, \mathbf{x})$ can be used instead of the smooth color function $\tilde{c}(t, \mathbf{x})$. Thus, Brackbill suggested for the volume force $\mathbf{f}_{\Gamma V}$

$$\mathbf{f}_{\Gamma V}(t, \mathbf{x}) = \sigma\kappa(t, \mathbf{x}) \frac{\nabla\rho(t, \mathbf{x})}{\rho_g - \rho_l} \; \frac{2\rho(t, \mathbf{x})}{\rho_g + \rho_l},$$

where the first fraction stands for the unit normal vector, and the second fraction ensures that the surface tension only depends on density gradients rather than on the value of the density itself. The main disadvantage of the CSF model is its non-conservative character, thus the conservation of momentum cannot be guaranteed during numerical simulations.

A conservative model has been developed by Lafaurie et al. [LNS+94] by discovering that the surface tension force can be represented as the divergence of a capillary stress tensor $\mathbf{T}_c$,

$$\mathbf{f}_{\Gamma V} = \nabla \cdot \mathbf{T}_c, \qquad \mathbf{T}_c = \sigma \left(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}\right) \delta(\phi). \tag{4.45}$$

The surface gradient defined in equation (4.15) can be reformulated as
$\nabla_\Gamma = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \cdot \nabla$.

In order to show that the representation (4.45) of the surface tension is reasonable, we consider for $\varphi \in \mathcal{D}(\mathbb{R})$

$$\begin{aligned}
\left(\nabla \cdot \left[\left(\mathbf{I} - \mathbf{n} \otimes \mathbf{n}\right) \delta(\phi)\right], \varphi\right) &= \left(\nabla\delta(\phi), \varphi\right) - \left(\nabla \cdot \left((\mathbf{n} \otimes \mathbf{n})\delta(\phi)\right), \varphi\right) \\
&= \left(\nabla\delta(\phi), \varphi\right) - \left((\nabla \cdot \mathbf{n})\delta(\phi)\mathbf{n}, \varphi\right) - \left(|\mathbf{n}|^2 \nabla\delta(\phi), \varphi\right) \\
&= \left(\kappa\delta(\phi)\mathbf{n}, \varphi\right).
\end{aligned}$$

We point out that in (4.45) the curvature κ does not appear explicitly. Lafaurie et al. also use a smoothed color function $\tilde{c}$, similar to the smoothed function of Brackbill. Thus, the resulting term for the surface tension is

$$\mathbf{f}_{\Gamma V} = \sigma\nabla \cdot \left(|\nabla\tilde{c}| \, \mathbf{I} - \frac{\nabla\tilde{c} \otimes \nabla\tilde{c}}{|\nabla\tilde{c}|}\right).$$

Discretizing a function containing a discontinuity, means that the corresponding jump takes place only in a few cells (resp. one cell). Thus, the problem in both described methods is that finite difference approximations are used for derivatives of these discretized functions, which can be inaccurate in certain situations.

In order to get an impression of the numerical errors that can accumulate during the computation of surface tension, the calculation of a spherical drop with zero velocity and at zero gravity is used as a classical example. In this situation, the drop should stay at rest with zero velocity field. Instead, the numerical errors, which results from the computation of the normal and the curvature, increase the amplitude of the velocity field. The arising currents are called *parasitic currents* or *spurious currents*. These spurious currents exists in many numerical methods treating interfaces. Dimensional analysis [LNS+94] shows that the magnitude $|\mathbf{u}_P|$ of the spurious currents depends on the surface tension coefficients σ and the dynamical viscosity μ and is given by

$$|\mathbf{u}_P| = C \, \frac{\sigma}{\mu}$$

where C is some constant. By numerical experiments Lafaurie et al. verify this law with $C \approx 0.01$. The magnitude $|\mathbf{u}_P|$ decreases by a factor of 2 or 4 by smoothing the color function. Scardovelli and Zaleski [SZ99] state that the dimensionless numbers *capillary number*, the *Laplace number*, and the *Weber number* could be used as criteria for the presence of spurious currents.

Several methods were developed to attenuate the spurious currents [Rud98], [MYS02], [PZ99], and [SP00]. The two main issues in order to reduce spurious currents are the coupling of the surface tension force with the flow solver and the accurate computation of the curvature [RR02], [LFSF04]. In [JTB02], Jamet, Torres and Brackbill stated that "the essential requirement for the elimination of parasitic currents is energy conservation. Strict momentum conservation does not appear to be essential."

In 2002, Renardy and Renardy [RR02] developed an accurate representation of the surface tension, which effectively reduces spurious currents. Their algorithm is known as *PROST: parabolic reconstruction of surface tension*. Instead of the smoothed color function used by Brackbill and Lafaurie, they calculate a least-squares fit of a quadratic surface to the color function for each cell and its neighbors. The probably most important characteristic of this method is that the algorithm converges spatially in contrast to its predecessors, i.e., the spurious currents attenuate with a higher refinement. For more details about this algorithm, we refer to [RR02].

Recently, Lörstad and Fuchs [LF04] present a procedure to reduce the spurious currents with second order accuracy. The main idea of their approach is to use a relatively simple model (in comparison to [RR02], [PAB$^+$97]) to compute the normal vector and the curvature. For the computation of the normal vector, they introduce a procedure which they call *direction averaged normal (DAN)*. In this procedure an initial normal vector is computed on the basis of a specially defined distance function. By means of this initial normal vector and its corresponding VOF-value f_0, a plane for this cell can be reconstructed. This plane corresponding to f_0 can be considered as a dividing plane of all adjacent cells (3^2 cells in 2D and 3^3 cells in 3D), i.e., this plane corresponds to a volume fraction field (of the adjacent cells) that may not be identical to the original VOF-field. By an iterative process the normal is adapted such that the volume fraction field corresponding to the plane and the original VOF-field corresponding to the interface are nearly identical. For the computation of the curvature they introduce the *direction averaged curvature (DAC)* model, which uses the improved normal vector from the DAN model and the same distance function with modified parameters (cells that are more than one cell away may be used), but the DAC approach requires no iteration procedure. Both methods are described in detail in [LFSF04] and [LF04].

4.3 Binary Droplet Collision: Experiment and Simulation

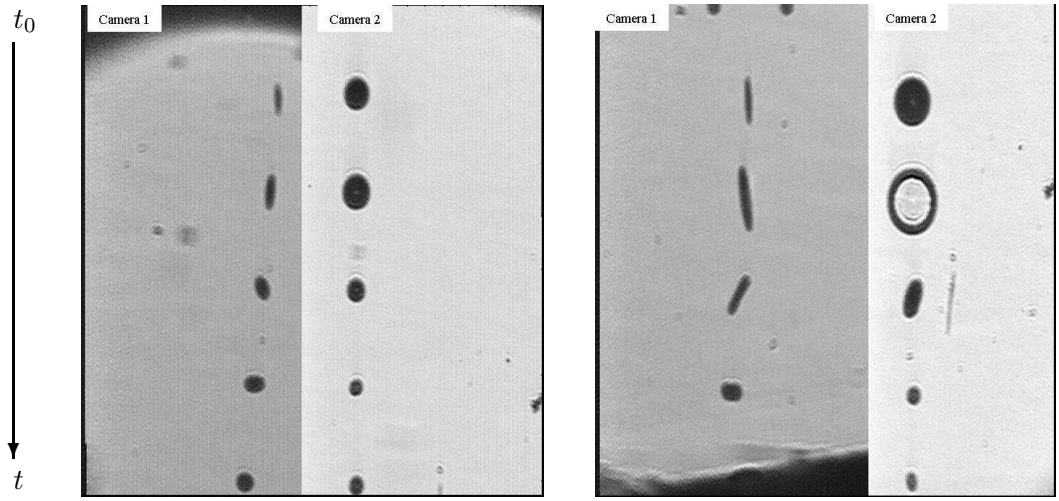
This section deals with the simulation of the flow behavior of a binary droplet collision using non-Newtonian fluids. We compare the numerical result with the corresponding experiment which was carried out by M. Motzigemba (University Paderborn) and N. Roth (University Stuttgart).

The non-Newtonian fluid was selected with respect to two criteria: high shear thinning effects and low elastic effects. Therefore, the behavior is assumed to be that of a generalized Newtonian fluid (see section 2.5.4). Actually, for the viscosity function which is used in the simulation, a local strong solution for system (3.2) exists (see chapter 3) due to theorem 3.3.1. Of course, this result is only valid for one-phase flows in the full space $\mathbb{R}^n$.

4.3.1 Experimental Setup

In order to demonstrate the differences between Newtonian and non-Newtonian flow behavior, we explain the experiment of a Newtonian droplet collision. The droplet collision is considered as central collision, i.e., the collision complex can be assumed to be symmetric.

In the experiment, glycerol (the macroscopic behavior is similar to water) for the Newtonian fluid and carboxymethylcellulose (CMC) (the material properties are similar to those of water, but the viscosity decreases with increasing shear rate) for the non-Newtonian fluid were used. Both fluids are characterized by similar values of the characteristic dimensionless groups (Weber and Reynolds number). As mentioned, the main property of the selected non-Newtonian fluid is the decreasing viscosity with increasing shear rate. For more details about the experiment we refer to [MRB$^+$02].



(a) Newtonian (b) Non-Newtonian

Figure 4.7: Experiment of a binary droplet collision [MRB$^+$02]. A sequence of photos is taken from two different positions at different points of time.

Two cameras took photos of the collision complex from two different positions. A sequence of photos at different points of time is shown in figure 4.7. The non-Newtonian fluid (see figure 4.7(b)) exposes the lowering viscosity during the droplet collision by a

larger maximum diameter of the generated collision complex and a very thin lamella arises, compared to the Newtonian collision (see figure 4.7(a)).

Figure 4.8 shows the measured shear viscosity $\mu(\dot{\gamma})$ in dependence of the shear rate $\dot{\gamma}$. For highest prescribed shear rate, the non-Newtonian fluid shows no region of constant viscosity. Therefore, the infinity-shear-rate viscosity is assumed to be zero and for the simulation of the viscosity function of the non-Newtonian fluid a modified Carreau model

$$\mu(\dot{\gamma}) = \frac{\mu_0}{1 + \frac{\mu_0}{K}\dot{\gamma}^{1-m}} \tag{4.46}$$

was selected. The zero-shear-rate viscosity of the non-Newtonian fluid is given by $\mu_0 = 102$ mPas, whereas the constants K and m have to be determined from the experimental data. By fitting the parameters K and m of the viscosity function (4.46), the experimental data and the theoretical curve correspond well for $K = 6.69$ kg/ms and $m = 0.8309$ (see figure 4.8).

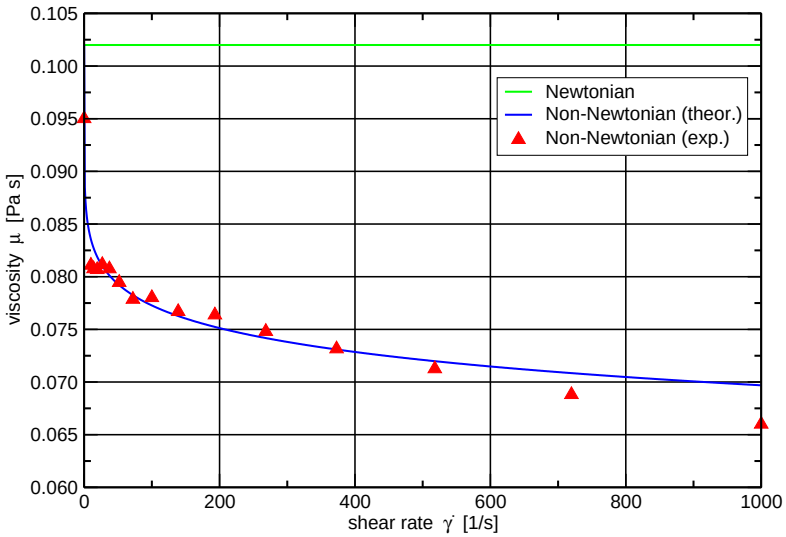


Figure 4.8: Viscosity of the experimental liquids: experimental values and fit curve for the modified Carreau model [MRB+02].

4.3.2 Admissibility of the Viscosity Function

In this section, the exponents m of the viscosity function (4.46) are determined for which a local strong solution exists for system (3.2). We are especially interested in the previously outlined case where $m = 0.8309$.

For the space dimension n theorem 3.3.1 shows local existence if the viscosity function

fulfills the following two conditions

$$\mu(s) \;>\; 0 \tag{4.47-a}$$

$$\mu(s) + 4\left(1 - \frac{1}{n}\right) s\,\mu'(s) \;>\; 0. \tag{4.47-b}$$

In chapter 3, we assumed that the viscosity functions depends on $\|\mathbf{D}\|^2$ and derived the above stated conditions under this assumption. However, since in fluid mechanics it is common to describe the viscosity function μ in dependence of the shear rate $\dot{\gamma}$, we set $\tilde{\mu}(\dot{\gamma}) = \mu(\|\mathbf{D}\|^2)$. Therefore, we rewrite the above conditions for the viscosity function $\tilde{\mu}$. Since $4\,\|\mathbf{D}\|^2 = 2\dot{\gamma}^2$ holds, we obtain

$$s = \|\mathbf{D}\|^2 = 1/2\;\dot{\gamma}^2.$$

Then, we get for the derivatives

$$\frac{\partial\tilde{\mu}(\dot{\gamma})}{\partial\dot{\gamma}} = \frac{\partial\mu(s(\dot{\gamma}))}{\partial\dot{\gamma}} = \dot{\gamma}\frac{\partial\mu(s)}{\partial s}.$$

Thus, the conditions (4.47) read as

$$\tilde{\mu}(\dot{\gamma}) \;>\; 0 \tag{4.48-a}$$

$$\tilde{\mu}(\dot{\gamma}) + 2\left(1 - \frac{1}{n}\right)\dot{\gamma}\,\tilde{\mu}'(\dot{\gamma}) \;>\; 0 \tag{4.48-b}$$

for the viscosity function $\tilde{\mu}$. In the following, we write again μ instead of $\tilde{\mu}$.

For the viscosity function (4.46), condition (4.48-a) is obviously satisfied and condition (4.48-b) yields

$$\mu(\dot{\gamma})\left[1 + C\left(2 - \frac{2}{n}\right)(m-1)\right] > 0 \text{ with } C := \frac{\frac{\mu_0}{K}\dot{\gamma}^{1-m}}{1 + \frac{\mu_0}{K}\dot{\gamma}^{1-m}}.$$

Thus, we get existence for

$$m > 1 - \frac{n}{C(2n-2)}$$

in dependence of the constant C. We are interested in the lowest upper bound for m. Thus, due to $0 < C < 1$, in the worst case we obtain

$$m > 1 - \frac{n}{2n-2}. \tag{4.49}$$

The case $C = 0$ corresponds to $\dot{\gamma} = 0$ such that both conditions (4.48-a) and (4.48-b) coincide.

For the 3D case with $n = 3$, we infer from inequality (4.49) that we get a local strong solution for system (3.2), if $m > 1/4$. Thus, we get local existence for the investigated fluid in the situation of theorem 3.3.1.

Computational Domain		$[0, 0.14] \times [0, 0.14] \times [0, 0.07]$			cm^3
Grid Resolution		$256 \times 256 \times 128$			
Initial Droplet	Radius	R_0	=	0.02729	cm
	Velocity	$\mathbf{u}_0$	=	$(0, 0, -495.5024)$	cm/s
Density	Droplet	ρ_l	=	1	g/cm^3
	Bulk Phase	ρ_g	=	0.0012	g/cm^3
Viscosity	Droplet	μ_0	=	1.02	$g/cm\ s$
	see eq. (4.46)	K	=	6.69	$g/cm\ s$
		m	=	0.8309	
	Bulk Phase	μ_g	=	0.00018	$g/cm\ s$,
Surface Tension Coefficient		σ	=	70	g/s^2

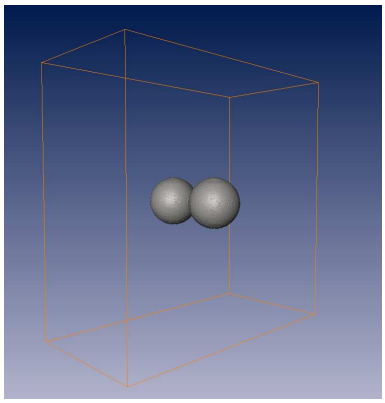
Table 4.1: Simulation Setup

4.3.3 Numerical Setup and Results

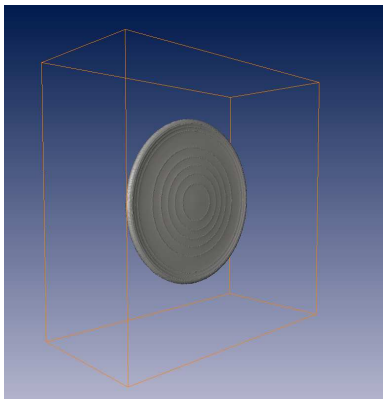
As mentioned before, the VOF-method is suitable to compute collisions of droplets, i.e., in case that two droplets are close together (up to one cell) the VOF- variable unites the two droplets. Since the collision complex is assumed as central collision with rotational symmetry, it is sufficient that we only compute one quarter of one droplet. Then, the whole collision complex can be reconstructed using the symmetries.

The data used for the simulation of the non-Newtonian droplet collision is collected in table 4.1. Concerning the simulation setup we mention that we used equidistant grids in each single space direction. The high refinement is necessary in order to resolve the very thin lamella of the collision complex and to obtain a circular impact. In figure 4.9, the simulation of the whole collision complex at different points of time is depicted, comparison with the experiment (see figure 4.7(b)) shows that both results qualitatively match with respect to the surface shape. In order to additionally obtain a quantitative comparison, we introduce the dimensionless time t^*, using the point in time corresponding to the initial impact as reference point. For both experiment and simulation, figure 4.10 shows the normalized diameter $D^* = d/D_0$ of the collision complex versus the dimensionless time $t^* = t/(D_0/U)$. Here, D_0 denotes the initial droplet diameter, i.e., $D_0 = 2R_0$ and U denotes the relative velocity which is given by twice the initial velocity $\mathbf{u}_0$, i.e., $U = 2\mathbf{u}_0$ (see table 4.1). In fact, we observe that the simulation reflects the same size of the collision complex as appearing in the experiment. The maximum diameter of the collision complex matches well, whereas the time scale of the collision complex contraction is overestimated. This effect can also be observed in the Newtonian collision as well as in bubble collisions [Koe04]. One reason could be that the non-Newtonian fluid used in the experiment contains some elastic parts which are not included in the simulation. Furthermore, we consider that the collision is a highly dynamic process occurring in only a few milliseconds. Thus, the possibility for even very small perturbations in the experiments can result in a distortion of the time scales.

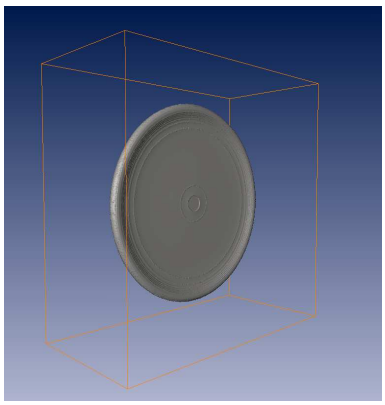
Numerical difficulties arose for the calculation of the very thin inner lamella of the collision complex (see figure 4.7(b)). Since the droplets move very fast, the initial impact



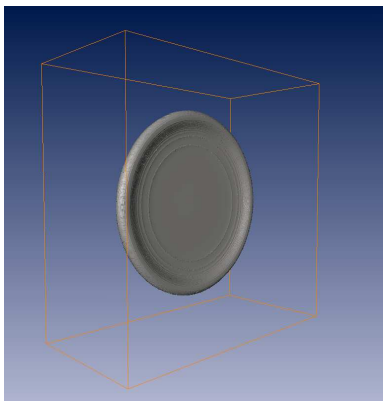
(a) $t = 0$



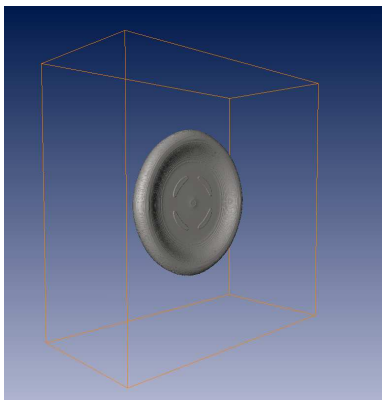
(b) $t = 0.2$ ms, $t^* = 3.13$



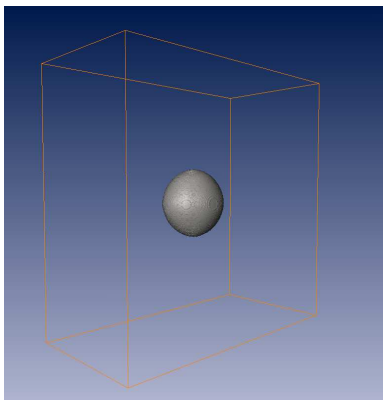
(c) $t = 0.4$ ms, $t^* = 6.76$



(d) $t = 0.6$ ms, $t^* = 10.39$



(e) $t = 0.8$ ms, $t^* = 14.03$



(f) $t = 1.15$ ms, $t^* = 20.38$

Figure 4.9: Simulation of the binary droplet collision using non-Newtonian fluids. Note that figure (a) with initial time $t = 0$ does not correspond to $t^* = 0$, since the reference point t^* corresponds to the initial impact.

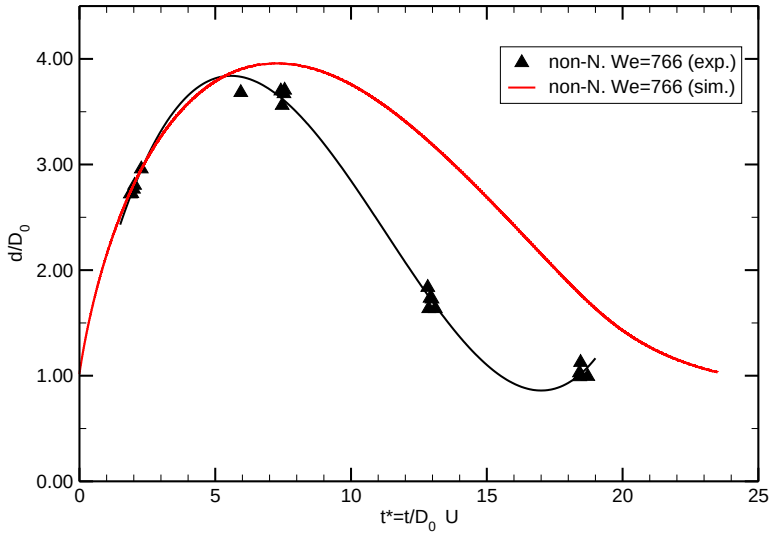


Figure 4.10: Collision Complex Diameter versus Time

is extremely high. At the same moment the fluid reaches the cell in the center of the collision complex, the fluid moves out of this cell towards the plane. However, numerical errors occurring in the center can disturb the collision complex in a way that the very thin lamella does not remain in one piece and gaps appear inside the lamella. This problem is explained by taking a closer look at the VOF-variable (see figure 4.11). In reality, the VOF variable should be 1 inside the whole droplet, but in the simulation some cells with false interfaces appear. Figure 4.11(a) represents the effect for a coarse resolution of the computation complex. However, in order to describe the impact of the collision corresponding to the experiment, we avoid the problem of such "air inclusions" by setting the defective values of the VOF-variable to one. This happens exactly once, and is carried out in a time step shortly after the initial impact. Evidently, the point in time for overwriting the values below 1 depends on the initial position of the droplet at time t_0.

According to (4.8) the Navier-Stokes equations are split up. Thus, the shear dependent viscosity (4.46) is incorporated in equation (4.8-b) which is usually solved via the finite volume method (4.12) with $\psi = \mathbf{u}$ and the flux $\mathbf{q} = \mathbf{S}$. Before the viscosity is computed via (4.46), the shear rate $\dot{\gamma}$ has to be determined. By definition of the shear rate

$$\dot{\gamma} = \left[4\left(\frac{\partial u_1}{\partial x_1}\right)^2 + 4\left(\frac{\partial u_2}{\partial x_2}\right)^2 + 4\left(\frac{\partial u_3}{\partial x_3}\right)^2 + 2\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right)^2 + 2\left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}\right)^2 + 2\left(\frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}\right)^2 \right]^{1/2},$$

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32
32	1	1	1	1	1	1	1	0.614	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31	1	1	1	1	1	1	1	0.997	0.266	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	1	1	1	1	1	1	1	1	0.809	0.011	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	1	1	1	1	1	1	1	1	1	0.333	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28	1	1	1	1	1	1	1	1	1	0.779	0.001	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	1	1	1	1	1	1	1	1	1	0.999	0.214	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26	1	1	1	1	1	1	1	1	1	1	0.578	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	1	1	1	1	1	1	1	1	1	1	0.909	0.019	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24	1	1	1	1	1	1	1	1	1	1	1	0.242	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23	1	1	1	1	1	1	1	1	1	1	1	0.514	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	1	1	1	1	1	1	1	1	1	1	1	0.772	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21	1	1	1	1	1	1	1	1	1	1	1	0.976	0.041	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20	1	1	1	1	1	1	1	1	1	1	1	1	0.223	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	1	1	1	1	1	1	1	1	1	1	1	1	0.407	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	1	1	1	1	1	1	1	1	1	1	1	1	0.572	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	1	1	1	1	1	1	1	1	1	1	1	1	0.722	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	1	1	1	1	1	1	1	1	1	1	1	1	0.861	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	1	1	1	1	1	1	1	1	1	1	1	1	0.982	0.013	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	1	1	1	1	1	1	1	1	1	1	1	1	1	0.115	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	1	1	1	1	1	1	1	1	1	1	1	1	1	0.224	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	1	1	1	1	1	1	1	1	1	1	1	1	1	0.323	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	1	1	1	1	1	1	1	1	1	1	1	1	1	0.414	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	1	1	1	1	1	1	1	1	1	1	1	1	1	0.503	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	1	1	1	1	1	1	1	1	1	1	1	1	1	0.597	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	1	1	1	1	1	1	1	1	1	1	1	1	1	0.708	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	1	1	1	1	1	1	1	1	1	1	1	1	1	0.846	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	1	1	1	1	1	1	1	1	1	1	1	1	1	0.987	0.039	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0.283	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0.667	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0.996	0.252	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0.905	0.055	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	0.797	0.766	0.836	0.865	0.666	0.997	1	1	1	1	1	1	1	1	1	1	0.5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

(a) VOF-variable at Time Step t_n.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32
32	1	1	1	1	1	1	1	0.506	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31	1	1	1	1	1	1	1	0.984	0.188	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	1	1	1	1	1	1	1	1	0.733	0.001	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	1	1	1	1	1	1	1	1	1	0.264	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28	1	1	1	1	1	1	1	1	1	0.716	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	1	1	1	1	1	1	1	1	1	0.994	0.162	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26	1	1	1	1	1	1	1	1	1	1	0.527	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	1	1	1	1	1	1	1	1	1	1	0.872	0.007	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24	1	1	1	1	1	1	1	1	1	1	1	0.207	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23	1	1	1	1	1	1	1	1	1	1	1	0.481	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	1	1	1	1	1	1	1	1	1	1	1	0.743	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21	1	1	1	1	1	1	1	1	1	1	1	0.964	0.029	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20	1	1	1	1	1	1	1	1	1	1	1	1	0.206	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	1	1	1	1	1	1	1	1	1	1	1	1	0.395	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	1	1	1	1	1	1	1	1	1	1	1	1	0.565	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	1	1	1	1	1	1	1	1	1	1	1	1	0.719	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	1	1	1	1	1	1	1	1	1	1	1	1	0.862	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	1	1	1	1	1	1	1	1	1	1	1	1	0.984	0.016	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	1	1	1	1	1	1	1	1	1	1	1	1	1	0.124	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	1	1	1	1	1	1	1	1	1	1	1	1	1	0.238	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	1	1	1	1	1	1	1	1	1	1	1	1	1	0.343	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	1	1	1	1	1	1	1	1	1	1	1	1	1	0.44	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	1	1	1	1	1	1	1	1	1	1	1	1	1	0.534	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	1	1	1	1	1	1	1	1	1	1	1	1	1	0.633	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	1	1	1	1	1	1	1	1	1	1	1	1	1	0.75	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	1	1	1	1	1	1	1	1	1	1	1	1	1	0.894	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	1	1	1	1	1	1	1	1	1	1	1	1	1	0.999	0.085	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0.352	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0.748	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0.352	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0.958	0.116	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0.62	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

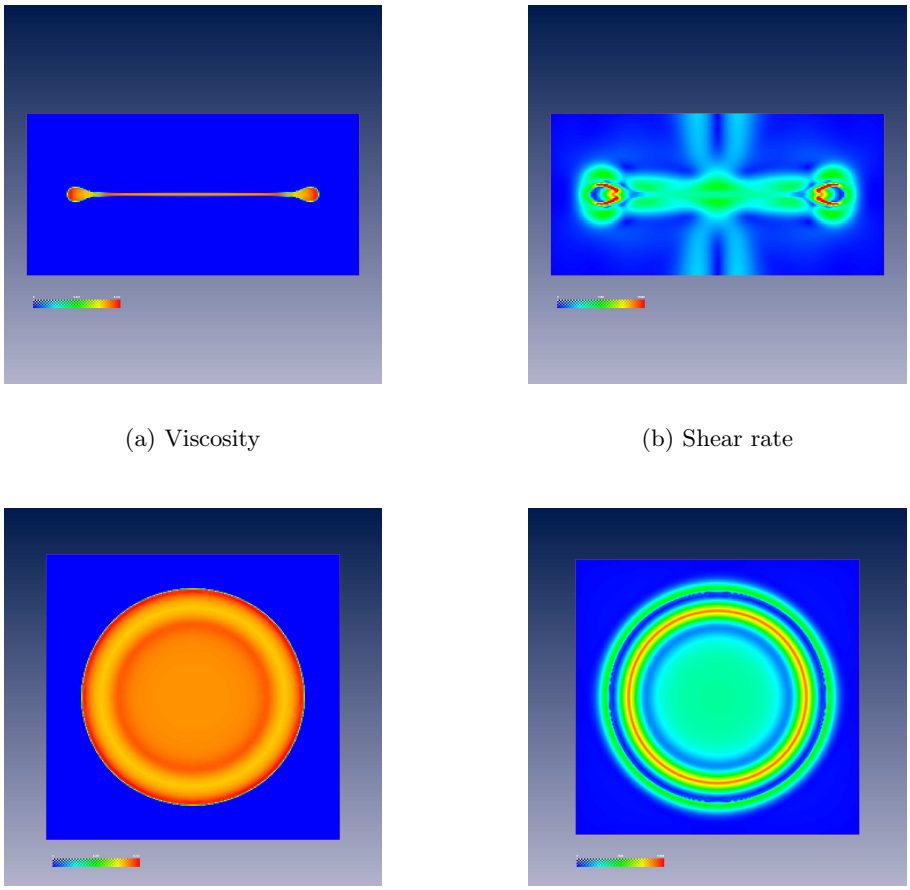
(b) VOF-variable at Time Step t_{n+1}.

Figure 4.11: Illustration of overwriting the VOF-variable of the non-Newtonian collision complex for an example of a coarse Grid. (a) shows the VOF-variable before and (b) after the overwriting.

holds, where the derivatives were approximated by central differences.

Next, we consider the viscosity and shear rate distribution inside the droplet collision complex. Figure 4.12 shows the comparison of the viscosity and shear rate distribution at time $t = 0.5$.

Comparing the distribution of viscosity and shear rate, we observe that the viscosity is high at those places where the shear rate is low. This corresponds to the desired effect of shear thinning. In figure 4.12(d), two rings of low shear rate emerge. This behavior can be understood by looking at figure 4.13. Thus, these rings of lower shear rate corresponds to the droplet shape.



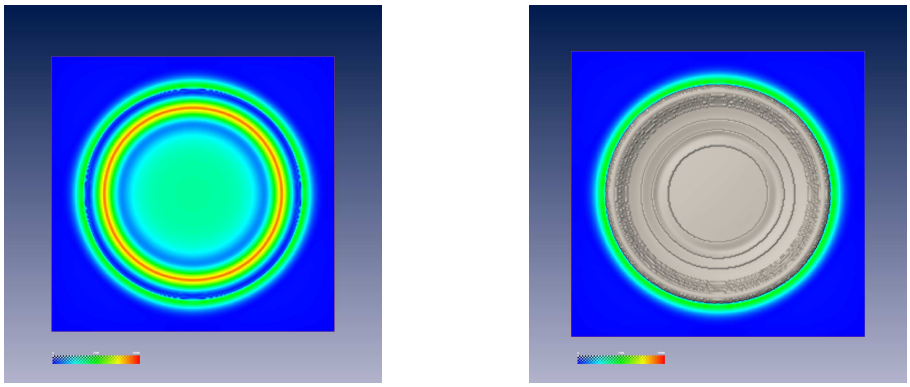
(a) Viscosity

(b) Shear rate

(c) Viscosity

(d) Shear rate

Figure 4.12: Comparison of the viscosity and shear rate distribution inside the droplet at time $t = 0.5$ ms, $t^* = 5.58$. The scale of the viscosity: *Blue*: $1.8E-4$ *Red*: 0.722 and of the shear rate: *Blue*: 0 *Red*: 15000



(a) Shear rate (b) Shear rate

Figure 4.13: Shear rate distribution in connection with the droplet shape at time $t = 0.5$.

4.4 Existence of Strong Solutions for Two Phase Flows

We conclude this chapter with an existence result for the free boundary value problem of the two-phase Navier-Stokes system with surface tension which is proved by Escher, Prüss, and Simonett [EPS03]. Two-phase Navier-Stokes equations with surface tension have also been investigated in [Tan93], [Tan95], [ID96], [Den00].

In this section, we distinguish the two fluid phases by the indices "+" and "-" instead of g and l in order to express the existence result in a more compact form and to conform with Escher et al. [EPS03].

Let $\Omega_\pm(t) \subset \mathbb{R}^{n+1}$, $n \geq 1$ be the domains occupied by Newtonian fluids at time t, $\Gamma(t) = \partial\Omega_\pm(t)$ denotes the boundary of $\Omega_\pm(t)$ with outer normal $\mathbf{n}(t, \mathbf{x})$ to Ω_+, where $\Omega_+(t) \cup \Gamma(t) \cup \Omega_-(t) = \mathbb{R}^{n+1}$.

Escher et al. studied the following problem (see system (4.36))

$$\begin{aligned}
\tfrac{\partial}{\partial t}(\rho_\pm \mathbf{u}) + \operatorname{div}(\rho_\pm \mathbf{u} \otimes \mathbf{u}) &= -\nabla p + \operatorname{div} \mathbf{S} \\
\operatorname{div} \mathbf{u} &= 0, \qquad t > 0, \quad \mathbf{x} \in \Omega_\pm(t) \\
\Gamma(0) = \Gamma_0, \qquad & \mathbf{u}(0, \mathbf{x}) = \mathbf{u}_0(\mathbf{x}), \qquad \mathbf{x} \in \Omega_\pm(0) \\
[-p\,\mathbf{n} + \mathbf{S}\mathbf{n}] = -\sigma\kappa(\Gamma(t))\mathbf{n}, \qquad & [\mathbf{u}] = 0 \\
V = \mathbf{u} \cdot \mathbf{n}, \qquad & t > 0, \quad \mathbf{x} \in \Gamma(t),
\end{aligned} \tag{4.50}$$

where the stress tensor $\mathbf{S}$ is given by $\mathbf{S} = 2\mu_\pm \mathbf{D}$ and $\mathbf{D}$ is the ordinary deformation tensor $\mathbf{D} = 1/2\left[\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right]$. The density $\rho_\pm$, the viscosity $\mu_\pm$, and the surface tension σ are assumed to be positive constants. As before, $\kappa(\Gamma(t))$ represents the mean curvature of $\Gamma(t)$, which is defined to be positive where $\Omega_+(t)$ is convex (locally), and

$V(t,\mathbf{x})$ means the normal velocity of $\Gamma(t)$, which is positive where $\Omega_+(t)$ is expanding. Furthermore, the bracket $[\Psi]$ denotes the jump of the quantity Ψ across the surface $\Gamma(t)$ (see equation (4.24)).

Furthermore, Escher et al. consider the situation that Γ_0 is close to a plane, say $\mathbb{R}^n$, i.e., Γ_0 is graph over $\mathbb{R}^n$ which is given by a function ρ_0 with $|\nabla\rho_0|_{L_\infty(\mathbb{R}^n)}$ small such that their main result reads as follows.

Theorem 4.4.1 *Fix $p > n+3$ and let $\rho_0 \in W_p^{3-2/p}(\mathbb{R}^n)$, $\mathbf{u}_0 \in W_p^{2-2/p}(\mathbb{R}^{n+1}\backslash\Gamma_0)$ be given. Assume that the compatibility conditions*

$$\operatorname{div}\mathbf{u}_0 = 0 \text{ on } \mathbb{R}^{n+1}\backslash\Gamma_0, \quad [\mathbf{S}_0\mathbf{n} - (\mathbf{n}\cdot\mathbf{S}_0\mathbf{n})\mathbf{n}] = 0, \quad [\mathbf{u}_0] = 0, \quad \text{on } \Gamma_0$$

are satisfied, where $\mathbf{S}_0 = 2\mu\mathbf{D}(\mathbf{u}_0)$.

Then, there exists $\eta > 0$ such that for $|\nabla\rho_0|_\infty < \eta$ there is $t_0 = t_0(\mathbf{u}_0,\rho_0) > 0$ and a unique classical solution $(\Gamma,\mathbf{u},p)$ of problem (4.50) on $(0,t_0)$. In addition, $\Gamma(t)$ is a graph over $\mathbb{R}^n$ given by $\rho(t)$

$$M = \bigcup_{t\in(0,t_0)} \{t\}\times\Gamma(t)$$

is a real analytic manifold, and with

$$\Omega := \big\{(t,\mathbf{x}',y) :\ t\in(0,t_0),\ \mathbf{x}'\in\mathbb{R}^n, y\neq\rho(t,\mathbf{x}')\big\}$$

the function $(\mathbf{u},p) : \Omega \to \mathbb{R}^{n+2}$ is real analytic.

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