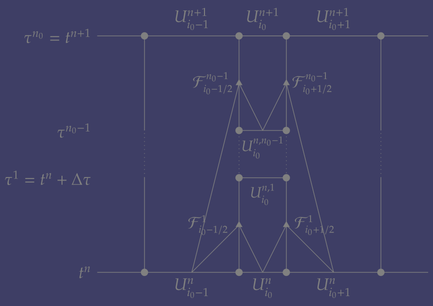
Results for Two Phase Flows with Phase Transition

Ferdinand Thein

$$\frac{\partial}{\partial t}\psi + \nabla_x \cdot (\psi \mathbf{v} + \boldsymbol{\phi}) = \xi,$$

$$\mathring{\psi}_S + \psi_S \left(\nabla_\alpha w_\tau^\alpha - 2\mathrm{K}_M w_\nu\right) + \nabla_\alpha \phi_\tau^\alpha = w_\nu \llbracket \psi \rrbracket - \llbracket \psi \mathbf{v} + \boldsymbol{\phi} \rrbracket \cdot \boldsymbol{\nu} + \xi_S$$



$$\begin{aligned}
\frac{\partial}{\partial t}\rho + \nabla_x \cdot (\rho \mathbf{v}) &= 0,\\
\frac{\partial}{\partial t}(\rho \mathbf{v}_i) + \nabla_x \cdot \left(\rho \mathbf{v}_i \mathbf{v} + p\mathbf{e}^{(\mathbf{i})}\right) &= 0,\ i \in \{1,2,3\},\\
\frac{\partial}{\partial t}\mathcal{E} + \nabla_x \cdot (\mathbf{v}(\mathcal{E} + p) + \mathbf{q}) &= 0,\\
\frac{\partial}{\partial t}(\rho s) + \nabla_x \cdot \left(\rho s \mathbf{v} + \frac{\mathbf{q}}{T}\right) &= \zeta \geq 0.
\end{aligned}$$

$$\mathbf{U}_{i_0}^{n,\nu+1} = \frac{\Delta x_{i_0}^{\nu}}{\Delta x_{i_0}^{\nu+1}} \mathbf{U}_{i_0}^{n,\nu} - \frac{\Delta \tau}{\Delta x_{i_0}^{\nu+1}} \left[\mathcal{F}_{i_0+\frac{1}{2}}^{\nu} - \mathcal{F}_{i_0-\frac{1}{2}}^{\nu}\right]$$

$$0 \leq \zeta_S = \left\llbracket \dot{m}\left(\frac{g_S}{T_S} - \frac{g}{T}\right) - \frac{1}{2T_S}\dot{m}\left(\mathbf{v} - \mathbf{w}\right)^2 \right\rrbracket + \left\llbracket \left(\frac{1}{T} - \frac{1}{T_S}\right)\left(\mathbf{q} \cdot \boldsymbol{\nu} + \dot{m}\left(g + Ts\right)\right) \right\rrbracket$$

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Zusammenfassung

Kompressible Zweiphasenströmungen sind von großem Interesse, sowohl in vielen Anwendung wie Wasserturbinen oder der chemischen Industrie, als auch in verschiedenen Forschungsgebieten wie der Meteorologie, den Ingenieurwissenschaften oder der Physik. Wir betrachten hier Strömungen von flüssigen und gasförmigen Phasen derselben Substanz und berücksichtigen dabei auch Phasenübergänge, d.h. Kondensation und Verdampfung. Bedingt durch die hohe Komplexität des betrachteten Problems ist es nötig Ergebnisse verschiedener Forschungsgebiete miteinander zu kombinieren, um weitere Erkenntnisse zu gewinnen. Deshalb berücksichtigen wir in dieser Arbeit die physikalische Modellierung, die mathematische Analysis und die numerische Behandlung von Zweiphasenstömungen. Der erste Teil der Arbeit stellt die benötigten Grundlagen zur Verfügung, Teil zwei behandelt ein isothermes Modell und abschließend wird in Teil drei ein adiabates Modell diskutiert.

Die drei Hauptresultate dieser Arbeit sind ein allgemeines Existenzresultat für ein Gleichungssystem, welches isotherme Zweiphasenstömungen modelliert, eine numerische Methode zum Lösen dieser Gleichungen, welche auch das Entstehen von Phasen behandeln kann und ein Resultat zur Nichtexistenz von Lösungen im Fall adiabater Zweiphasenströmungen. Die Ergebnisse für den isothermen Fall werden in Teil zwei gezeigt und das Resultat für die Nichtexistenz in Teil drei.

Um die verschiedenen Fragestellungen zu verstehen und mögliche Antworten zu erarbeiten, benötigen wir Resultate der Thermodynamik und ein Verständnis der beschreibenden Bilanzgleichungen. Wir werden uns deshalb nicht einfach darauf beschränken die entsprechenden Ergebnisse zu zitieren, sondern eine etwas detailiertere Einführung in diese Themen geben. Der erste Teil der vorliegenden Arbeit gibt deshalb einen Überblick der wesentlichen zu Grunde liegenden Konzepte. Das erste Kapitel stellt eine kompakte Behandlung der Gleichgewichtsthermodynamik dar. Wir erklären die verschiedenen thermodynamischen Potentiale und die zugehörigen Maxwell-Relationen. Diese werden in der anschließenden Einführung von Zustandsgleichungen benötigt. Die Zustandsgleichungen haben einen wesentlichen Einfluss auf die Dynamik der betrachteten Systeme. Mit einer kurzen Darstellung der Thermodynamik für zwei Phasen beenden wir das erste Kapitel.

Eine Herleitung allgemeiner Bilanzgleichungen, in der Gegenwart von Flächen über welche die betrachteten Größen unstetig sein können, wird im zweiten Kapitel gegeben. Insbesondere die Bilanzgleichungen für diese singulären Flächen sind hier von besonderem Interesse. Im wesentlichen findet man diese Herleitung auch in der Literatur, jedoch werden dabei einige Details weggelassen. Wenn man sich aber neu in dieses Gebiet einarbeitet, ist diese Art der Präsentation möglicherweise zu kurz gehalten. Deshalb kann die hier vorliegende Präsentation auch als Einstieg in diese Thematik genutzt werden. Wir beenden das Kapitel mit einer kompakten Darstellung der Theorie hyperbolischer partieller Differentialgleichungen mit Fokus auf den Euler-Gleichungen.

Der zweite Teil der Arbeit behandelt Zweiphasenströmungen, welche durch die isothermen Euler-Gleichungen beschrieben werden. Im dritten Kapitel beweisen wir ein allgemeines Existenzresultat für das dazu gehörende Riemann-Problem. Hier beschreiben wir die Strömung durch einen Satz Euler-Gleichungen und eine Zustandsgleichung, welche sowohl die flüssige als auch die gasförminge Phase beschreibt. Der Massenfluss zwischen den Phasen ist durch eine kinetische Relation gegeben. Wir zeigen die Existenz für alle thermodynamisch sinnvollen Zustandsgleichungen, sowohl für zweiphasige als auch einphasige Anfangsdaten. Für Anfangsdaten die aus einer Phase bestehen berücksichtigen wir Nukleation und Kavitation. Wir möchten betonen, dass die Phasen sowohl in stabilen als auch in metastabilen Zuständen vorliegen können und die Phasen müssen sich nicht im mechanischen Gleichgewicht befinden.

Im anschließenden vierten Kapitel behandeln wir das Problem numerisch und geben eine Methode an, die auch die Entstehung von Phasen berücksichtigt.

In Anbetracht der Ergebnisse des zweiten Teils stellt sich die Frage, wie diese auf den Fall des vollen Systems von Euler-Gleichungen übertragen werden können. Diese Frage wird im dritten Teil beantwortet. Im ersten Teil ist ersichtlich geworden, dass der volle Satz Euler-Gleichungen keinen Wärmefluss enthält und deshalb bezeichnen wir das System genauer als System adiabatischer Euler-Gleichungen. Im fünften Kapitel wird nun der Einfluss unterschiedlicher Annahmen an der Phasengrenze auf die Struktur der Lösung des Riemann-Problems untersucht. Hierbei stellt sich heraus, dass im Fall der klassischen Sprungbedingungen an der Phasengrenze kein Phasenübergang zwischen den reinen Phasen stattfinden kann. Deshalb müssen zusätzliche Größen, welcher auf der Phasengrenze definiert sind, mit einbezogen werden. Dies führt zum Verlust der selbstähnlichen Struktur der Lösung und wir erhalten eine Singularität auf der Phasengrenze.

Im abschließenden sechsten Kapitel zeigen wir die Nichtexistenz von Kondensation durch Kompression und Verdampfung durch Expansion zwischen den reinen Phasen für Modelle, die auf den adiabaten Euler-Gleichungen basieren.

Zusammenfassend zeigen die Ergebnisse der vorliegenden Arbeit, dass der Wärmefluss für die Beschreibung von Zweiphasenströmungen unbedingt mit einbezogen werden muss. In den isothermen Eulergleichungen ist der Wärmefluss indirekt noch vorhanden, nur dass die Energiegleichung hier zur Bestimmungsgleichung für den Wärmefluss wird. Im isothermen Fall führt dies gewissermaßen zu einer unendlich schnellen Ausbreitung der Wärme. In den adiabaten Gleichungen ist der Wärmefluss jedoch nicht vorhanden. Aus diesem Grund können die isothermen Eulergleichungen, im Vergleich mit den adiabaten Eulergleichungen, als geeignetes Modell zu Beschreibung von Zweiphasenströmungen mit Phasenübergängen angesehen werden.

Summary

Compressible two phase flows are a topic of high interest in many applications such as water turbines or chemical engineering and different areas of current research such as meteorology, engineering and physics. In particular we consider liquid/vapor flows of a single substance and we take phase transitions between the two phases into account, i.e. condensation and evaporation. Due to the complexity of the problem one needs to combine different fields of research to gain further insight. Therefore this work partly covers the physical modeling, the analytical investigation and the numerical treatment of two phase flows. The first part provides the basis for this work, the second part treats an isothermal model and the third part discusses an adiabatic model.

The three main results of this work are a general existence result for a system of equations modeling isothermal two phase flows, a numerical method for the isothermal case that is able to treat phase creation and a nonexistence result for the case of adiabatic two phase flows. The results for the isothermal case are presented in the second part and the nonexistence result is given in the third part.

In order to establish these results we need the theory of thermodynamics together with an understanding of the governing equations, i.e. the balance laws. Instead of simply giving the needed results, we believe that a detailed introduction is more suited for a better understanding of the problems considered. Therefore the first part of this thesis is dedicated to the introduction of the main concepts. The first chapter gives a compact survey of equilibrium thermodynamics. We give the different thermodynamic potentials and the corresponding Maxwell relations. These results are needed in the subsequent discussion of equations of state which have a crucial impact on the dynamics of the systems considered. We close the first chapter with a brief introduction of thermodynamics for two phases.

In the second chapter we derive local balance laws in the presence of interfaces across which quantities may be discontinuous. A special focus is given to the balance laws for quantities on such an interface. To some extent this derivation may be found in the literature, but quite often several details of the calculation are left out. For researchers new to this topic, this kind of presentation might be rather short. Thus the derivation in the

present work may serve as a good introduction to this topic. We first derive general balance laws which are then specified for certain quantities and corresponding assumptions. We close the second chapter with a brief introduction to hyperbolic conservation laws with a focus on the Euler equations.

The second part treats the case of a two phase flow which is governed by the isothermal Euler equations. In chapter three we give a general existence result for the corresponding Riemann problem. Here we use one set of Euler equations for both phases together with one equation of state which covers the liquid as well as the vapor region of the substance considered. The mass transfer is modeled using a kinetic relation. We show the existence for all thermodynamically reasonable equations of state for two phase initial data as well as for single phase initial data. In the case of single phase initial data the solution may exhibit phase creation, i.e. nucleation or cavitation. We want to highlight that this result also covers phase transitions away from equilibrium and the phases are allowed to be in a stable or a metastable state.

In the fourth chapter we discuss how the isothermal problem may be solved numerically. The method suggested can treat the two phase case as well as phase creation. Several examples are presented at the end of the second chapter.

From the second part the question arises whether the results obtained may be extended to the full Euler system or not. This question is answered in the third part. From the first part we know that the heat flux is missing in the full Euler system and thus we refer to them as the adiabatic Euler equations. In chapter five we discuss the influence of different assumptions at the phase boundary on the solution structure of the Riemann problem for the adiabatic Euler equations. It turns out that in the case of the classical jump conditions at the phase boundary, no interface quantities, there can be no phase transition between pure phases. Therefore additional quantities of the interface have to be considered, since we have excluded the heat flux. With this assumption we lose the self-similar solution structure and obtain a solution with a singularity on the phase boundary.

The final chapter six contains a nonexistence result which highlights the observations of the previous chapter. In particular we show that condensation by compression and evaporation by expansion between pure phases is not possible for various models relying on the adiabatic Euler equations.

Thus the results of this thesis strongly recommend the consideration of the heat flux in two phase flow problems. The heat flux is still included in the isothermal Euler equations. Here the energy equation decouples from the system and determines the heat flux. In the isothermal case one might say that the heat is distributed at infinite speed. In contrast, in the adiabatic case the heat flux is absent. Hence the isothermal Euler equations, compared to the adiabatic Euler equations, may serve as a good model for two phase flow problems with phase transition.

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Reaching this further milestone would not have been possible without my caring family. My parents always supported my sister, brother and me in

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[1] "Eulergleichungen mit Phasenübergängen.", HA 6471/2 – 1

every aspect. It is their foundation I started from. I truly want to thank Anna and Leo for sticking together as siblings. You were a great support all the time.

Most importantly my deepest love and gratitude belong to my wife Julia. The past years have been so intense and exciting with starting jobs, becoming parents and getting married. You knew when I needed some time for math and most important you recognized when I needed a break to keep the balance. The times spent together with our wonderful daughter Leonore belong to the best in my life and provided so much fun and energy. I will always appreciate your trust, love and support.

Contents

Part I

Concepts

Introduction

It is an often recognized pattern that certain mathematical problems arise from applications, then they emancipate somehow and become important mathematical topics on their own. Nevertheless even in these situations mathematicians try to find analogies to the underlying (physical) concepts in order to establish a theory suited to fully understand the considered problems. This is exactly what happened in the field of fluid dynamics. Scientist tried to develop a theory in order to describe fluid phenomena and were faced with severe mathematical difficulties. It then turned out that these difficulties are in some sense deep mathematical problems, of which many are still open.

The main results of the present work deal with such problems involving selected aspects of fluid dynamics. In particular we are concerned with liquid and vapor phases of a single substance and investigate their dynamics under different conditions such as a fixed temperature. Therefore it is necessary to equip the reader with all concepts that are needed throughout this thesis to establish our results. To this end we mainly provide two things. On the one hand we will focus on the physical aspects that are needed to provide the models and their theoretical bases. On the other hand there is of course the mathematical theory which kind of certifies the physical models. By establishing a mathematical framework for the physical models, the theory will for example allow us to say in what sense we may expect solutions. Thus it helps to study the intrinsic structure of the given models. Since this is a mathematical thesis we want to give some priority to the physical aspects, because we belief that a thorough discussion of the physical principles is most helpful for understanding and solving the mathematical problems. We further assume that most of the readers are familiar with basic concepts of the analysis of partial differential equations and thus refer to the given literature apart from the presented results. According to the previous remarks the first part consists of two chapters.

Chapter 1 entitled *Thermodynamics* contains a compressed introduction of (equilibrium) thermodynamics. This chapter does not replace a deep study of this topic but merely serves as a guide through this field and thus presents the main results. Additionally we present certain calculations in detail where we are of the opinion that they are often of interest in everyday work but left out in the literature (due to the technical character). Further for readers not familiar with thermodynamics these additional calculations might serve as guiding examples to treat a wide range of thermodynamic problems mathematically.

Chapter 2 covers a wide range of topics with *Balance Laws* as the thematic parentheses. Some parts of Chapter 2 may be interpreted as the *non-equilibrium* extension of the results presented in Chapter 1. We will present a derivation of the local forms of a generic balance law in the presence of singularities. From these generic equations we obtain all the governing equations needed in this work. Further we observe how they are related and how they may be extended in certain situations. The main reason for this focus is that we think that this topic is quite difficult to get into and we thus additionally made some slight changes compared to the literature which we will comment as they appear. The chapter closes with a brief overview on the theory of *hyperbolic partial differential equations*.

The first part of this work consists of the two following chapters

- First, in Chapter 1 we will briefly present all thermodynamic results needed throughout this work.
- In Chapter 2 the conservation and balance laws that will describe the fluid motion will be derived and discussed.

1 Concepts: Thermodynamics

Presenting thermodynamics is perhaps one of the more difficult things throughout this thesis. In the book by Müller and Müller [65] the authors note at the very beginning that

> *Thermodynamics is the much abused slave of many masters [. . .].*

What they are missing in the following (surely non-exhaustive) listing is the mathematician investigating models and objects derived from thermodynamical principles. Since we do so we have another perspective on this field than for example the engineer working on cooling systems. Therefore we want to apologize to every physicist for not presenting every important name or idea as it is usually the case.

A brief summary of the thermodynamic results needed for the remaining work, would probably leave some readers puzzled due to the missing background and motivation of the results. Additionally more experienced readers may argue that fundamental concepts and connections between the relations are missing.

If in contrast the topic would be presented in all its generality, to give as much insight as possible, the chapter would cover some few hundred pages. This of course is way beyond the scope of this work. Nevertheless, since thermodynamics plays a crucial role throughout this thesis we want to present this topic in more detail. Therefore we will highlight the main results needed here and further present some calculations in detail which might be of interest for people new to this field of research.

For more details on thermodynamics we recommend the standard literature and the references therein. In particular we used the famous textbook by Landau and Lifshitz [51], as mentioned earlier [65], Rebhan [70] and

Bartelmann et al. [5]. Additionally we like to draw the readers attention to the following works. First we want to mention the lecture notes by Evans [27] (or the condensed version [29]) with a very nice introduction and description of the mathematical structure of thermodynamics and further references. Second the work by Lieb and Yngvason [57], where they present an axiomatic approach to the Second Law of thermodynamics. Finally we recommend the work by Menikoff and Plohr [60]. This article contains are very compact, yet detailed description of thermodynamics with a special focus on the Riemann problem for hyperbolic conservation laws.

The chapter is organized as follows. In Section 1.1 basic quantities, concepts and the *laws of thermodynamics* are introduced. The following Section 1.2 gives an overview of the different *thermodynamic potentials* and there connections, i.e. the *Maxwell relations*. These relations are of great importance for the mathematical treatment of thermodynamics. In Section 1.3 we introduce the concept of an *equation of state* which connects the theory with applications. In the two Subsections 1.3.1 and 1.3.2 we will discuss particular equations of state in more detail. These examples may serve the reader as guidelines when other equations of state need to be discussed. We finish this chapter with Section 1.4 containing a brief summary of aspects of the thermodynamics of different phases. In particular we are interested in equilibrium conditions, the *Maxwell construction* and thermodynamics of a surface.

We want to close this introduction with a remark on equilibrium and non-equilibrium thermodynamics. The results in the following chapter rely on the assumption that the considered system is in equilibrium or that the processes evolve in such a way that they can be considered as a sequence of connected equilibrium states. Based on this assumptions a theory was developed which is capable of dealing with many different questions arising in the field of thermodynamics. However, the question that remained was what to do if the system is far away from thermodynamic equilibrium. One example that comes up (especially in the context of this work) is the presence of different phenomena in fluid dynamics, such as shock waves or phase transitions. This question opened a field of research which is still of great interest. Some of the aspects will be covered in Chapter 2 which also contains helpful references.
Nevertheless the ideas and concepts of the equilibrium thermodynamics serve as the basis and key ingredient for the treatment of non-equilibrium

phenomena. This is best highlighted by an approach often made in non-equilibrium thermodynamics, i.e. it is assumed that a small part of a thermodynamic system is in equilibrium whereas the whole system does not need to be in equilibrium. Such a system is said to be in *local equilibrium*. Thus the results obtained in Chapter 1 may be applied to such systems. It remains to give some kind of criteria that tell us when a system allows such approximation. A precise quantification is given in the book of Mauri [59] which we will not present here in detail. Just to give an impression, it is for example stated that for a system consisting of gas a temperature gradient up to 10^4 K/cm still allows the assumption of local equilibrium. In Bedeaux et al. [8] even a temperature gradient of 10^6 K/cm is mentioned. These results serve as kind of justification to assume that we always have a system in local equilibrium in the context of this work, underlining the importance of the equilibrium results.

1.1 The Laws of Thermodynamics

Every system consisting of matter obeys the laws of thermodynamics. Precisely a *thermodynamic system* is a macroscopic amount of matter that, in an adequate sense, is delimited from its environment. Further it can be completely described by macroscopic variables. One may consider different types of systems which may also be described by different variables [1], e.g.

- *isolated systems* exclude the exchange of energy and matter. Therefore the energy is conserved and in equilibrium it is described by the *number of particles* N, the occupied *volume* V and the *internal energy* E.

- *Closed systems* allow energy exchange but forbid exchange of matter. The macroscopic equilibrium state is described by N, V and the *temperature* T.

- *Open systems* allow the exchange of energy and matter. In equilibrium they are described by V, T and the *chemical potential* μ.

The quantities we use may be distinguished in two categories. First we have the *state quantities* (or sometimes variables/parameters). State quantities describe a macroscopic system independent from the way it got there.

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[1] In this work we will use SI – units. Hence we have for the volume $[V] = \mathrm{m}^3$, the temperature $[T] = \mathrm{K}$ the energy $[E] = \mathrm{J} = \mathrm{Nm} = \mathrm{kgm}^2\mathrm{s}^{-2}$ and the chemical potential $[\mu] = \mathrm{Jmol}^{-1}$.

Mathematically speaking, state quantities are quantities which can be written as *exact differentials*, e.g. [5, 54]. These state quantities are either *intensive* or *extensive*. Extensive state quantities are proportional to the amount of the substance considered, such as energy, volume and entropy. Intensive properties do not depend on the amount of substance, just like temperature, pressure or densities of extensive quantities. Second we have the *process quantities* which (as the name indicates) describe the way how a system reaches a certain macroscopic state. Hence they are in general no exact differentials. Examples are the change of heat or the work done to or by the system. By *thermodynamic equilibrium* we understand a state

- that is unique, independent of its history and can be characterized by a finite number of macroscopic variables,
- which does not change as time evolves,
- where no macroscopic transport processes (e.g. mass) take place.

Now we skip quite a bit and state the three (or four, depending on how you count) laws of thermodynamics. The Zeroth Law of thermodynamics basically defines an equivalence relation for thermodynamic systems.

Zeroth Law of Thermodynamics 1.1.1. *Whenever two systems are in thermal equilibrium with a third one, these two are also in thermal equilibrium.*

The First Law of thermodynamics connects the process quantities heat and work to the state quantity internal energy[2]. It is also referred to as the impossibility of a *perpetual motion machine of first kind*[3].

First Law of Thermodynamics 1.1.2. *The sum of the differential heat δQ supplied to the system and the differential work done to the system δW give the differential of the internal energy* $\mathrm{d}E$*, i.e.*

$$\mathrm{d}E = \delta Q + \delta W.$$

The internal energy is determined up to some additive constant.

Mathematically the First Law ensures the existence of a twice differentiable function called internal energy E. Further E is an extensive state

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[2] $[Q] = [W] = [E] = \mathrm{J}$

[3] A perpetual motion machine of first kind is a virtual, *periodic* working machine which *solely* performs work. In particular it reaches its initial state after one cycle without losing energy.

variable and thus dE is an exact differential, cf. [27]. Note that this property of E holds regardless of the fact that δQ and δW may each be process dependent.

The Second Law of thermodynamics can be approached on two ways. First we have the phenomenological and second the statistical approach. Before we state the second law we want to give a notion of reversible and irreversible processes. A process is called *irreversible* if it cannot be undone in a way such that there are no permanent changes in the environment. If a process can be reversed without abiding changes to the environment it is called *reversible*. Now from a phenomenological point of view the Second Law comprises the observation that there are processes in nature which are allowed by the First Law but nevertheless do not occur. It is also referred to as the impossibility of a *perpetual motion machine of second kind*[4] [5].

Second Law of Thermodynamics 1.1.3. *For thermodynamic systems in equilibrium exists a state quantity called* entropy, S[6], *which for changes in reversible processes is given by*

$$\mathrm{d}S = \frac{\delta Q}{T}.$$

For irreversible processes in closed systems from one equilibrium state to another the entropy increases.

Again, mathematically the Second Law states that under certain circumstances there exists an integrating factor $1/T$ for δQ such that dS is an exact differential. This does not depend on the number of independent variables $X_1, \ldots, X_m$. The second part of the Second Law 1.1.3 can be summarized by *Clausius' inequality*

$$T\mathrm{d}S \geq \delta Q. \tag{1.1}$$

The equality only holds for reversible processes. As mentioned earlier the Second Law can also be derived from statistical considerations. Without going into too much details the statistical version states

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[4] A perpetual motion machine of second kind is a virtual, *periodic* working machine. During one cycle it absorbs heat and *completely* converts it into work without abiding changes in its environment.

[5] This formulation goes back to Planck. There are other formulations by Clausius and Kelvin. These formulations are all equivalent.

[6] $[S] = \mathrm{JK}^{-1}$

> *If a macroscopic system is not in equilibrium, the most likely change is an increase of entropy.*

Here the term *most likely* means *almost sure, apart from fluctuations*. For more details on the Second Law we refer to the afore mentioned literature, especially [57]. The First and Second Law of thermodynamics, especially the differential relations defined within, will be the ones we will use the most for deriving mathematical relations between different state quantities.

What is left missing by the First and Second law is some information about the limit as the temperature approaches zero [7]. Hence to complete the laws of thermodynamics we finally give the Third Law although it is not necessary for our purposes.

Third Law of Thermodynamics 1.1.4. *The entropy S of a thermodynamic system in equilibrium converges to a unique value for $T \to 0$. This is independent from the realized physical path and other state variables. Hence one is free to choose $S|_{T=0} = 0$.*

Since the Third Law is not relevant in our case we will not go into much details. Just note that the absolute value $T = 0\,\mathrm{K}$ cannot be realized and for justification of the Third Law quantum mechanical arguments are needed. See the literature mentioned before.

1.2 Thermodynamic Potentials and Maxwell Relations

Now with the laws of thermodynamic at hand we can exploit the formal structure that helps to investigate specific questions. A thermodynamic system in equilibrium can be described by extensive variables $(X_0, X_1, \dots, X_m) \in \Omega \subset \mathbb{R}^{m+1}$ which are independent from another. [8]. It is always possible to choose these variables such that the entropy is not among them and we have for the internal energy that $E = X_0$. The remaining variables may have different meanings, such as volume V or mole number N. We assume Ω to be an open and convex subset of $\mathbb{R}^{m+1}$ and call it state space. From now on

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[7] It is worth noting, that the existence of an absolute temperature scale is non trivial. Usually it is derived using Carnot cycles which implies the use of 1.1.2 and 1.1.3.

[8] It is a non trivial assumption that a system in equilibrium may be described by a finite number of variables and we again refer to the given literature (e.g. [70]).

we assume, if not stated otherwise, that all thermodynamic functions are defined and evaluated in Ω and conversely all states are taken such that they are within the domain of a thermodynamic function.
By the second law we know that there exists a function S called entropy. The entropy is a twice differentiable function

$$S : \Omega \to \mathbb{R} \quad \text{with} \quad S = S(E, X_1, \ldots, X_m). \tag{1.2}$$

This equation is called *fundamental equation* and contains all the information about a thermodynamic system. Further S has the following properties

(i) S is concave

(ii) $\partial S/\partial E = 1/T > 0$

(iii) S is positively homogeneous of degree one, i.e. $S(\lambda X) = \lambda S(X)$ for $\lambda > 0$

In [57] it is noted (as *Entropy principle*) that the Second Law 1.1.3 includes additivity of the entropy and also property (iii). Both together imply concavity (i), cf. [5], [27] or [57]. Following [57] the concavity (i) is then the key ingredient to show that $\partial S/\partial E$ exists (as already noted above). The fact that one can write (ii) is due to the fact that for two systems in thermal equilibrium the corresponding derivatives of the entropy with respect to the energy are equal. Consequently the temperatures of systems in equilibrium are equal. The fact that the Temperature is strictly positive[9] is a necessity for the existence of systems in equilibrium, see [51]. Now property (ii) always allows us to uniquely solve the fundamental equation (1.2) for E

$$E = E(S, X_1, \ldots, X_m). \tag{1.3}$$

Since (1.3) is only a reformulation of (1.2) it contains the same information and thus both can be considered to be equivalent. Further, following from the entropy properties, the internal energy has the following properties

(i) E is convex

(ii) $\partial E/\partial S = T > 0$

(iii) E is positively homogeneous of degree one, i.e. $E(\lambda X) = \lambda E(X)$ for $\lambda > 0$

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[9] For examples of negative Temperatures see §73 in [51].

Extensive Parameter X	Intensive parameter P
volume	pressure
mole number	(neg.) chemical potential
length	tension
area	surface tension
electric charge	electric force
magnetization	magnetic intensity

Table 1.1: Different examples for relations of extensive and intensive quantities related to E, taken from [27]

Note that for the moment it is obvious what is meant by $\partial S/\partial E$ or $\partial E/\partial S$ from a mathematical point of view. Nevertheless in thermodynamics it is common to keep the notation of a quantity (e.g. S) although it might be expressed by different variables. This is done since the physical meaning of a quantity does not change along a variable transformation. So to be precise one writes in our case

$$\frac{\partial S}{\partial E} = \left(\frac{\partial S}{\partial E}\right)_{X_1,\ldots,X_m} .$$

The notation on the right gives the information which physical function is the dependent and with respect to which variable are we evaluating the derivative. Outside the brackets one notes the remaining independent variables held constant. Instead of noting the variables held constant it is also common to note the type of process which is considered. For example if a certain derivative is evaluated for an adiabatic ($\delta Q = 0$) process. Note that the derivative of the extensive quantity E with respect to the extensive quantity S gives the intensive quantity T. A similar relation holds for the extensive variables $X_1, \ldots, X_m$, i.e. we can assign an intensive variable to every extensive variable. We define so called *generalized forces* or *energetic intensive quantities* as

$$P_i = -\left(\frac{\partial E}{\partial X_i}\right)_{S,X_1,\ldots,X_m \neq X_i}, \quad i = 1, \ldots, m.$$

There are several different possibilities for such quantities, see the non-exhaustive summary in Table 1.1. If we now write down the exact differential of the internal energy E we obtain

$$\mathrm{d}E = T\mathrm{d}S - \sum_{i=1}^{m} P_i \mathrm{d}X_i. \tag{1.4}$$

and vice versa for the entropy S

$$\mathrm{d}S = \frac{1}{T}\mathrm{d}E + \frac{1}{T}\sum_{i=1}^{m} P_i \mathrm{d}X_i. \tag{1.5}$$

Using the property (iii) (E positive homogeneous) we can use *Euler's homogeneous function theorem* and obtain for E (analogue for S)

$$E(S, X_1, \dots, X_m) = S\left(\frac{\partial E}{\partial S}\right)_{X_1,\dots,X_m} + \sum_{i=1}^{m} X_i \left(\frac{\partial E}{\partial X_i}\right)_{S,X_1,\dots,X_m \neq X_i} = TS - \sum_{i=1}^{m} P_i X_i. \tag{1.6}$$

Note here, that we made explicit use of the extensive character of the internal energy. Now since $\mathrm{d}E$ should be an exact differential due to the First Law 1.1.2 we have the following relations between the mixed second order derivatives

$$\left(\frac{\partial T}{\partial X_i}\right)_{S,X_1,\dots,X_m \neq X_i} = \left(\frac{\partial P_i}{\partial S}\right)_{X_1,\dots,X_m} \quad \text{and} \quad \left(\frac{\partial P_i}{\partial X_k}\right)_{S,X_1,\dots,X_m \neq X_k} = \left(\frac{\partial P_k}{\partial X_i}\right)_{S,X_1,\dots,X_m \neq X_i} \tag{1.7}$$

Similar relations are also obtained for the entropy S. These relations are called *Maxwell relations*. As we will see in a short moment there are further Maxwell relations derived from other state quantities. Now with all this at hand we want to introduce further thermodynamic potentials. Therefore we will use the *Legendre transform*, see for example [28, 89]. One motivation for this is the simple need for measurable quantities. For example, it would be convenient to know the internal energy in terms of the measurable quantities temperature and pressure instead of the volume and the not directly measurable entropy. For the following we set $X_1 = V > 0$, fix the remaining variables $X_2, \dots, X_m$ and simply write $E(S, V)$ or $S(E, V)$ respectively. As noted before the *pressure* p is given by

$$p = -\left(\frac{\partial E}{\partial V}\right)_S \quad \text{with} \quad [p] = \mathrm{Pa} = \mathrm{Nm}^{-2}.$$

A more detailed derivation can be found for example in [51] (see §12). Finally we can introduce additional thermodynamic potentials as Legendre transforms of the internal Energy.

Definition 1.2.1 (Thermodynamic Potentials)**.**

*(i) The **Helmholtz free energy** F is given by*

$$F(T,V) = \inf_S (E(S,V) - TS). \tag{1.8}$$

*(ii) The **enthalpy** H is given by*

$$H(S,p) = \inf_V (E(S,V) - pV). \tag{1.9}$$

*(iii) The **Gibbs energy** or **free enthalpy** G is given by*

$$G(T,p) = \inf_{(S,V)} (E(S,V) + pV - TS). \tag{1.10}$$

*The functions E, F, G, H are called **thermodynamic potentials***

For the physical interpretation of these potentials we refer to the given literature. So far we only used convexity of $E(S,V)$, but from now on we will assume *strict convexity* of $E(S,V)$. Therefore each infimum in Definition 1.2.1 is attained at a unique point and thus we can write the thermodynamic potentials as

$$F(T,V) = E(S,V) - TS,^{10} \text{ with } T = \left(\frac{\partial E}{\partial S}\right)_V, \tag{1.11}$$

$$H(S,p) = E(S,V) + pV, \text{ with } p = -\left(\frac{\partial E}{\partial V}\right)_S, \tag{1.12}$$

$$G(T,p) = E(S,V) + pV - TS, \text{ with } T = \left(\frac{\partial E}{\partial S}\right)_V, p = -\left(\frac{\partial E}{\partial V}\right)_S. \tag{1.13}$$

These potentials are equivalent to (1.3) considering the information about a system[11], see [70]. From now on we will assume that E is strictly convex

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[10] To be precise, here $S = S(T,V)$ solves $T = \frac{\partial E}{\partial S}(S,V)$. A similar remark applies to the other potentials.

[11] We consider exemplary the Helmholtz energy. First solve $\left(\frac{\partial F}{\partial T}\right)_V (T,V) = -S(T,V)$ for $T(S,V)$. Second, use (1.11) to obtain $E(S,V) = F(T(S,V),V) + T(S,V)S$.

with respect to (S, V) and S is strictly concave, respectively. Further we can derive the differentials for the other thermodynamic potentials. Exemplary we present the free energy F

$$\begin{aligned} \mathrm{d}F &\overset{(1.11)}{=} \mathrm{d}(E - TS) = \mathrm{d}E - S\mathrm{d}T - T\mathrm{d}S \overset{(1.4)}{=} T\mathrm{d}S - p\mathrm{d}V - S\mathrm{d}T - T\mathrm{d}S \\ &= -S\mathrm{d}T - p\mathrm{d}V. \end{aligned} \tag{1.14}$$

Identifying (1.14) with

$$\mathrm{d}F = \left(\frac{\partial F}{\partial T}\right)_V \mathrm{d}T + \left(\frac{\partial F}{\partial V}\right)_T \mathrm{d}V$$

gives the first derivatives (which also can be obtained using the chain rule in (1.11))

$$\left(\frac{\partial F}{\partial T}\right)_V = -S \quad \text{and} \quad \left(\frac{\partial F}{\partial V}\right)_T = -p. \tag{1.15}$$

For the enthalpy H one obtains

$$\mathrm{d}H = T\mathrm{d}S + V\mathrm{d}p, \tag{1.16}$$

$$\left(\frac{\partial H}{\partial S}\right)_p = T \quad \text{and} \quad \left(\frac{\partial H}{\partial p}\right)_S = V$$

and for the Gibbs energy

$$\mathrm{d}G = -S\mathrm{d}T + V\mathrm{d}p, \tag{1.17}$$

$$\left(\frac{\partial G}{\partial T}\right)_p = -S \quad \text{and} \quad \left(\frac{\partial G}{\partial p}\right)_T = V.$$

We want to make the reader aware of a further useful relation that exists between the internal energy and the Gibbs energy. Consider the internal energy to be determined by the entropy S, the volume V and the mole numbers N_j, $j = 1, \dots, n$ with $[N_j] = \text{mol}$. Equation (1.6) gives the famous *Gibbs–Duhem relation*

$$E = TS - pV + \sum_{j=1}^{n} \mu_j N_j \quad \overset{(1.13)}{\Leftrightarrow} \quad G = \sum_{j=1}^{n} \mu_j N_j. \tag{1.18}$$

The μ_j are the so called *chemical potentials* of the substances and if we only consider one pure substance we get

$$G = \mu N.$$

Since all these quantities are exact differentials we know that the mixed second order derivatives must be equal. This gives further Maxwell relations

$$\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial p}{\partial S}\right)_V, \tag{1.19}$$

$$\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial p}{\partial T}\right)_V, \tag{1.20}$$

$$\left(\frac{\partial T}{\partial p}\right)_S = \left(\frac{\partial V}{\partial S}\right)_p, \tag{1.21}$$

$$\left(\frac{\partial S}{\partial p}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_p. \tag{1.22}$$

Other relations can be obtained if we consider general coordinate transformations in two dimensions, which is quite often the case in thermodynamics. Assume we have the coordinates (x, y) and we apply a unique and smooth transformation (a diffeomorphism between two subsets of $\mathbb{R}^2$), such that we obtain (x, z). Here the new coordinate can be expressed as $z = z(x, y)$ and we can also invert it to obtain $x = x(y, z)$. Hence the *Jacobian* of $f(y, z) = (x(y, z), z)$ is

$$\mathbf{D}f = \frac{\partial(x,z)}{\partial(y,z)} = \begin{pmatrix} \frac{\partial x}{\partial y} & \frac{\partial x}{\partial z} \\ \frac{\partial z}{\partial y} & \frac{\partial z}{\partial z} \end{pmatrix} = \begin{pmatrix} \frac{\partial x}{\partial y} & \frac{\partial x}{\partial z} \\ 0 & 1 \end{pmatrix}.$$

Now we use the chain rule and apply it to our transformation and obtain

$$\frac{\partial(x,z)}{\partial(y,z)} = \frac{\partial(x,z)}{\partial(x,y)} \frac{\partial(x,y)}{\partial(y,z)}.$$

Taking the determinant on both sides gives

$$\left(\frac{\partial x}{\partial y}\right)_z = -\left(\frac{\partial z}{\partial y}\right)_x \left(\frac{\partial x}{\partial z}\right)_y. \tag{1.23}$$

This relation is also known as *Barkhausen's formula*

1.3 Equations of State

In the previous Section 1.2 we noted that equation (1.3) contains all the thermodynamical information about a system. An immediate question for example is what if the entropy is replaced by the (well measurable) temperature and we therefore have $E = E(T, X_1, \dots, X_m)$? If we use the second property of the internal energy ($T = \partial E/\partial S$) we obtain a partial differential equation for E but we need further information to yield a unique solution. The same can be observed for any other intensive variable. If the fundamental equation (1.3) is known one can obtain $m+1$ equations relating the intensive and extensive quantities, i.e.

$$\begin{aligned} T &= T(S, X_1, \dots, X_m), \\ P_i &= P_i(S, X_1, \dots, X_m),\ i = 1, \dots, m. \end{aligned}$$

These kind of equations are called *equations of state (EOS)*. The existence of $m+1$ EOS is secured by the thermodynamic laws. Combining these $m+1$ equations one may obtain further EOS and if for example all extensive variables are eliminated we can express the temperature as $T = T(P_1, \dots, P_m)$. But the equations of state need to be obtained empirically or statistically since they crucially depend on the considered system. Recall equation (1.6), it only contains the same information as equation (1.3) if we know all EOS. This fact can be seen as follows, from (1.6) we derive

$$\mathrm{d}E = T\mathrm{d}S + S\mathrm{d}T - \sum_{i=1}^{m} P_i \mathrm{d}X_i - \sum_{i=1}^{m} X_i \mathrm{d}P_i.$$

Now we subtract (1.4) and obtain

$$0 = S\mathrm{d}T - \sum_{i=1}^{m} X_i \mathrm{d}P_i. \tag{1.24}$$

Now suppose all m EOS for the P_i are known. Further we use that T and the P_i are state quantities

$$\begin{aligned} \mathrm{d}T &= \left(\frac{\partial T}{\partial S}\right)_{X_1,\dots,X_m} \mathrm{d}S + \sum_{i=1}^{m} \left(\frac{\partial T}{\partial X_i}\right)_{S,X_1,\dots,X_m \neq X_i} \mathrm{d}X_i, \\ \mathrm{d}P_i &= \left(\frac{\partial P_i}{\partial S}\right)_{X_1,\dots,X_m} \mathrm{d}S + \sum_{j=1}^{m} \left(\frac{\partial P_i}{\partial X_j}\right)_{S,X_1,\dots,X_m \neq X_j} \mathrm{d}X_j,\ i = 1, \dots, m \end{aligned}$$

and thus obtain together with (1.24)

$$\begin{aligned}\left(\frac{\partial T}{\partial S}\right)_{X_1,\ldots,X_m} &= -\frac{1}{S}\sum_{i=1}^{m} X_i \left(\frac{\partial P_i}{\partial S}\right)_{X_1,\ldots,X_m \neq X_i}, \\ \left(\frac{\partial T}{\partial X_i}\right)_{S,X_1,\ldots,X_m \neq X_i} &= -\frac{1}{S}\sum_{j=1}^{m} X_j \left(\frac{\partial P_j}{\partial X_i}\right)_{S,X_1,\ldots,X_m \neq X_j}, \quad i = 1,\ldots,m.\end{aligned}$$

Finally T can be obtained by integration up to a constant. Note that equation (1.24) is also called *Gibbs–Duhem relation* as well as (1.18). The most common situation is that we know something about the pressure, the volume and the temperature, i.e. a relation $f(p,V,T) = 0$. This relation is an *incomplete* EOS since it is lacking information of the system. The relation $p = p(V,T)$ is called *thermal* EOS. If we combine it with a *caloric* EOS $E = E(V,T)$ we regain the complete picture, see [5] or [60]. Therefore the last missing pieces are the *response functions* or *material laws*. These response functions are directly measurable quantities. For our purposes we only need five of them and due to the Maxwell relations there are only three of them independent.

Definition 1.3.1 (Response Functions)**.**

(i) Heat capacity[12] *at constant volume:*
$C_V = T\left(\frac{\partial S}{\partial T}\right)_V$ *with* $[C_V] = \mathrm{JK}^{-1}$

(ii) Heat capacity at constant pressure: $C_p = T\left(\frac{\partial S}{\partial T}\right)_p$ *with* $[C_p] = \mathrm{JK}^{-1}$

(iii) Coefficient of thermal expansion: $\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p$ *with* $[\alpha] = \mathrm{K}^{-1}$

(iv) Isothermal compressibility: $\kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T$ *with* $[\kappa_T] = \mathrm{Pa}^{-1}$

(v) Adiabatic (isentropic) compressibility: $\kappa_S = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_S$ *with* $[\kappa_S] = \mathrm{Pa}^{-1}$

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[12] In general heat capacities are defined as $C_x = \left(\frac{\delta Q_{rev}}{\mathrm{d}T}\right)_X$ Here X is a state parameter (e.g. constant magnetic field) held constant during a reversible heat exchange, cf. [5].

It is worth noting that second order derivatives of thermodynamic potentials can always be written in terms of directly measurable quantities, see [60]. Measuring these quantities one may obtain the thermal and caloric EOS and using the Maxwell relations then gives the fundamental equation. How this can be done is explained for example in [65].
The following Lemma 1.3.2 collects some results that will be used later on. The proof will also be given to demonstrate some typical manipulations using thermodynamic relations.

Lemma 1.3.2. *Consider the response functions as given in Definition 1.3.1. Then the following results hold.*

(i) $C_V = \left(\frac{\partial E}{\partial T}\right)_V$ *and* $C_p = \left(\frac{\partial H}{\partial T}\right)_p$.

(ii) $C_p \geq C_V > 0$.

(iii) $\frac{\kappa_S}{\kappa_T} = 1 - \frac{\alpha^2 V T}{C_p \kappa_T} = \frac{C_V}{C_p}$.

Proof:

(i) The first statement is obvious since it directly follows using the chain rule for the potentials $E = E(S(T,V),V)$ and $H = H(S(T,p),p)$.

(ii) Let us first consider the Gibbs energy (1.13). Since we may express $V = V(T,p)$ we can use the Helmholtz energy (1.11) and write

$$G(T,p) = F(T,V(T,p)) + pV(T,p).$$

Using (1.15) we obtain

$$\left(\frac{\partial G}{\partial T}\right)_p = \left(\frac{\partial F}{\partial T}\right)_V \quad \text{and} \quad \left(\frac{\partial^2 G}{\partial T^2}\right)_p = \left(\frac{\partial^2 F}{\partial T^2}\right)_V + \frac{\partial F}{\partial T \partial V}\left(\frac{\partial V}{\partial T}\right)_p. \qquad (+)$$

This gives

$$\begin{aligned} \frac{C_p - C_V}{T} &\overset{1.3.1}{=} \left(\frac{\partial S}{\partial T}\right)_p - \left(\frac{\partial S}{\partial T}\right)_V \overset{(1.15)}{=} -\left(\frac{\partial^2 G}{\partial T^2}\right)_p + \left(\frac{\partial^2 F}{\partial T^2}\right)_V \\ &\overset{(+)}{=} -\frac{\partial F}{\partial T \partial V}\left(\frac{\partial V}{\partial T}\right)_p \overset{(1.15)}{=} \left(\frac{\partial p}{\partial T}\right)_V \left(\frac{\partial V}{\partial T}\right)_p \\ &\overset{(1.23)}{=} -\left(\frac{\partial V}{\partial T}\right)_p^2 \left(\frac{\partial p}{\partial V}\right)_T \overset{1.3.1}{=} \frac{\alpha^2 V}{\kappa_T} \geq 0. \end{aligned}$$

For the positivity we use the convexity of the internal energy

$$\frac{1}{V\kappa_T} = -\left(\frac{\partial p}{\partial V}\right)_T = \left(\frac{\partial^2 F}{\partial V^2}\right)_T = \left(\frac{\partial^2 E}{\partial V^2}\right)_S - \left(\frac{\partial^2 E}{\partial S \partial V}\right)^2 \left(\frac{\partial E}{\partial S}\right)_V^{-1} \geq 0.$$

(iii) The second equality follows from the equation $C_p - C_V = \frac{\alpha^2 VT}{\kappa_T}$ in the proof of (ii). Hence we only prove $\frac{\kappa_S}{\kappa_T} = \frac{C_V}{C_p}$.

$$\begin{aligned}
\kappa_S &= -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_S \overset{(1.23)}{=} \frac{1}{V}\left(\frac{\partial S}{\partial p}\right)_V \left(\frac{\partial V}{\partial S}\right)_p \\
&= \frac{1}{V}\left(\frac{\partial S}{\partial T}\right)_V \left(\frac{\partial T}{\partial S}\right)_V \left(\frac{\partial S}{\partial p}\right)_V \left(\frac{\partial V}{\partial T}\right)_p \left(\frac{\partial T}{\partial V}\right)_p \left(\frac{\partial V}{\partial S}\right)_p \\
&= \frac{1}{V}\left(\frac{\partial S}{\partial T}\right)_V \left(\frac{\partial T}{\partial p}\right)_V \left(\frac{\partial V}{\partial T}\right)_p \left(\frac{\partial T}{\partial S}\right)_p \\
&\overset{(1.23)}{=} -\frac{1}{V}\left(\frac{\partial S}{\partial T}\right)_V \left(\frac{\partial V}{\partial p}\right)_T \left(\frac{\partial T}{\partial V}\right)_p \left(\frac{\partial V}{\partial T}\right)_p \left(\frac{\partial T}{\partial S}\right)_p \overset{1.3.1}{=} \kappa_T \frac{C_V}{C_p}.
\end{aligned}$$

□

Lemma 1.3.2 (iii) immediately shows that only three of the five quantities are independent. For our later purposes we therefore follow Menikoff and Plohr and define dimensionless quantities as in [60].

Definition 1.3.3 (Dimensionless Quantities)**.** *Given a thermodynamic system described by the fundamental equation $E(S,V)$ the following dimensionless quantities can be defined:*

(i) The adiabatic exponent *or synonymous the* dimensionless sound speed

$$\gamma = \frac{V}{p}\left(\frac{\partial^2 E}{\partial V^2}\right)_S = \frac{1}{p\kappa_S}. \tag{1.25}$$

(ii) The Grüneisen coefficient

$$\Gamma = -\frac{V}{T}\left(\frac{\partial^2 E}{\partial S \partial V}\right) = \frac{\alpha V}{C_V \kappa_T}. \tag{1.26}$$

(iii) The dimensionless specific heat

$$g = \frac{pV}{T^2}\left(\frac{\partial^2 E}{\partial S^2}\right)_V = \frac{pV}{C_V T}. \tag{1.27}$$

(iv) The fundamental derivative

$$\mathcal{G} = -\frac{1}{2}V\frac{\left(\frac{\partial^3 E}{\partial V^3}\right)_S}{\left(\frac{\partial^2 E}{\partial V^2}\right)_S} = -\frac{1}{2}V\frac{\left(\frac{\partial^2 p}{\partial V^2}\right)_S}{\left(\frac{\partial p}{\partial V}\right)_S}. \tag{1.28}$$

Analogously for an isothermal process

(i) The (isothermal) dimensionless sound speed

$$\gamma_T = -\frac{V}{p}\left(\frac{\partial p}{\partial V}\right)_T = \frac{1}{P\kappa_T}. \tag{1.29}$$

(ii) The (isothermal) fundamental derivative

$$\mathcal{G}_T = -\frac{1}{2}V\frac{\left(\frac{\partial^2 p}{\partial V^2}\right)_T}{\left(\frac{\partial p}{\partial V}\right)_T}. \tag{1.30}$$

If it is clear from the context the subscript T in the isothermal case is omitted.

These dimensionless quantities are very helpful in discussing the Riemann problem for the Euler equations. Further they have several useful interpretations which we will not present here in detail. We therefore again highly recommend [60] and just present some remarks. Every additional property that we need will be given by the time it is needed.

Remark 1.3.4.

(i) Systems with a convex fundamental equation are called thermodynamically stable.

(ii) The convexity of $E(S,V)$ *can be expressed in terms of* g, γ *and* Γ*, i.e.*

$$E(S,V) \text{ convex} \quad \Leftrightarrow \quad g \geq 0, \gamma \geq 0 \text{ and } g\gamma \geq \Gamma^2. \tag{1.31}$$

(iii) The thermodynamic laws do not confine the sign of $\mathcal{G}$*.*

(iv) In the isothermal case one degree of freedom is fixed and hence the corresponding condition for the convexity of E is $\gamma_T \geq 0$*. Note that there is the following relation*

$$\frac{\gamma_T}{\gamma} = \frac{C_V}{C_p}. \tag{1.32}$$

(v) If $\Gamma \neq 0$ *one can choose p and V as independent variables.*

(vi) Considering (V,T) *as independent variables one obtains for* γ *and* $\mathcal{G}$

$$\gamma = -\frac{V}{p}\left[\left(\frac{\partial p}{\partial V}\right)_T - \frac{T}{C_V}\left(\frac{\partial p}{\partial T}\right)_V^2\right] = -\frac{V}{p}\left(\frac{\partial p}{\partial V}\right)_T + \frac{\Gamma^2}{g}, \tag{1.33}$$

$$\begin{aligned}\mathcal{G} = \frac{V^2}{2p\gamma}\Bigg[&\left(\frac{\partial^2 p}{\partial V^2}\right)_T - \frac{3T}{C_V}\left(\frac{\partial p}{\partial T}\right)_V\left(\frac{\partial^2 p}{\partial V \partial T}\right) \\ &+ \frac{3T}{C_V^2}\left(\frac{\partial p}{\partial T}\right)_V^2\left(\frac{\partial C_V}{\partial V}\right)_T + \frac{T}{C_V^2}\left(\frac{\partial p}{\partial T}\right)_V^3\left(1 - \frac{T}{C_V}\left(\frac{\partial C_V}{\partial T}\right)_V\right)\Bigg].\end{aligned} \tag{1.34}$$

We want to close this general introduction with the definition of the sound speed, since it is most important for the treatment of fluid dynamics.

Remark 1.3.5 (Specific Quantities)**.** *So far extensive quantities were denoted by capital letters*[13]*, which should emphasize the dependence on the amount or mass of the substance. Quite often it is very useful to consider* specific *quantities, i.e. per amount of substance or per mass. In this case the extensive quantities become intensive and we therefore will use the corresponding small letter. Which case is considered is often clear from the name of the new variable, e.g.* specific volume *with* $[v] = \mathrm{m^3kg^{-1}}$ *or* molar volume *with* $[v_m] = \mathrm{m^3mol^{-1}}$*. If not stated otherwise we will only consider specific quantities* per mass *in this work. The differential relations obtained so far remain valid in contrast for example to formula (1.6), see [27].*

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[13] The temperature being an exception.

Definition 1.3.6 (Sound Speed). *The sound speed a*[14] *is given by*

$$a = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s} = \sqrt{-v^2\left(\frac{\partial p}{\partial v}\right)_s}. \tag{1.35}$$

Here ρ denotes the mass density*, v the* specific volume *with $v = 1/\rho$ and s the specific entropy. For isothermal processes the sound speed is given by*

$$a_T = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_T} = \sqrt{-v^2\left(\frac{\partial p}{\partial v}\right)_T}. \tag{1.36}$$

A detailed motivation of this definition can be found for example in [52]. Since v and s are not that convenient in some applications, we want to give further formulas for the sound speed using different choices of variables

Lemma 1.3.7. *Given the sound speed defined by (1.35) and further assume that a smooth transformation of the thermodynamic variables can be applied. Then the sound speed can be written in terms of the new thermodynamic variables (x, y) as*

$$a^2 = -v^2\left(\frac{\partial p}{\partial x}\right)_y\left(\frac{\partial x}{\partial v}\right)_s - v^2\left(\frac{\partial p}{\partial y}\right)_x\left(\frac{\partial y}{\partial v}\right)_s. \tag{1.37}$$

In particular the following relations hold

(i) for (v, T)

$$a^2 = -v^2\left(\frac{\partial p}{\partial v}\right)_T + \frac{v^2 T}{c_v}\left(\frac{\partial p}{\partial T}\right)_v^2,$$

(ii) for (v, e) with e being the specific internal energy[15]

$$a^2 = -v^2\left(\frac{\partial p}{\partial v}\right)_e + pv^2\left(\frac{\partial p}{\partial e}\right)_v,$$

(iii) for (p, v)

$$a^2 = v^2\left(\frac{\partial e}{\partial p}\right)_v^{-1}\left(\left(\frac{\partial e}{\partial v}\right)_p + p\right).$$

---

[14] $[a] = \mathrm{ms}^{-1}$

[15] This constellation is very important when using conservative variables for the Euler equations.

Proof: Equation (1.37) is just the chain rule applied to (1.35). The formula for the case (v, T) follows from (1.37) together with (1.20), (1.23) and 1.3.1 . The case (v, e) also follows directly from (1.37). In the third case we want to use (p, v) as independent variables and hence we cannot use (1.37). First we consider the internal energy to be given in (p, v)

$$\mathrm{d}e = \left(\frac{\partial e}{\partial p}\right)_v \mathrm{d}p + \left(\frac{\partial e}{\partial v}\right)_p \mathrm{d}v.$$

This expression is inserted in the differential for the (specific) entropy

$$\mathrm{d}s = \frac{1}{T}\mathrm{d}e + \frac{p}{T}\mathrm{d}v = \frac{1}{T}\left(\frac{\partial e}{\partial p}\right)_v \mathrm{d}p + \frac{1}{T}\left(\left(\frac{\partial e}{\partial v}\right)_p + p\right)\mathrm{d}v.$$

From the requirement $s = const.$ we finally obtain

$$\begin{aligned} 0 = \mathrm{d}s &= \frac{1}{T}\left(\frac{\partial e}{\partial p}\right)_v \mathrm{d}p + \frac{1}{T}\left(\left(\frac{\partial e}{\partial v}\right)_p + p\right)\mathrm{d}v \\ \Leftrightarrow \quad \mathrm{d}p &= \underbrace{-\left(\frac{\partial e}{\partial p}\right)_v^{-1}\left(\left(\frac{\partial e}{\partial v}\right)_p + p\right)}_{=-a^2/v^2}\mathrm{d}v. \end{aligned}$$

□

As already mentioned before, one often has an EOS and needs the corresponding thermodynamic potentials and other related quantities. In the following we therefore want to present several different EOS and their associated potentials and quantities.

1.3.1 Ideal Gas and Stiffened Gas EOS

The presumably most popular EOS is the *ideal gas* EOS. It can be derived from phenomenological thermodynamics as well as from statistical considerations. Experiments by *Boyle*, *Mariott* and *Gay-Lussac* led to the ideal gas laws

(i) $pV = const.$ for $T = const.$

(ii) $p \propto T$ for $V = const.$

(iii) $V \propto T$ for $p = const$.

Of further importance is *Avogadro's Law* (see [65]):

> *Equal volumes of different gases at the same pressure and temperature contain equally many particles.*

Altogether these laws are reflected in the ideal gas EOS

$$pV = Nk_BT. \tag{1.38}$$

Here $k_B = 1.38065 \cdot 10^{-23}\,\mathrm{JK}^{-1}$ denotes the *Boltzmann constant*. There are other equivalent versions of this law using relations between the universal constants. In fact by using the *universal gas constant* $R = 8.3145\,\mathrm{JK}^{-1}\mathrm{mol}^{-1}$ and *Avogadro's constant* $N_A = 6.02214129 \cdot 10^{23}\,\mathrm{mol}^{-1}$ we obtain

$$pV = Nk_BT = N\frac{R}{N_A}T = nRT. \tag{1.39}$$

Here $n = N/N_A$ denotes the *amount of substance* with $[n] = \mathrm{mol}$. If we consider the density $\rho = Nm_A/V$ where m_A denotes the mass[16] of a single molecule (or atom in the case of Helium for example) we can also write

$$p = \rho\frac{k_BT}{m_A}. \tag{1.40}$$

Although this (thermal) EOS is not complete, in the sense discussed previously, one can already draw several conclusions.

Proposition 1.3.8. *The following statements hold for an ideal gas (1.39).*

(i) C_p *and* C_V *only depend on the temperature.*

(ii) $C_p - C_V = nR$.

(iii) The internal energy only depends on the temperature and is given by

$$E(T) = \int_{T_r}^{T} C_V(\tau)\,\mathrm{d}\tau + E_r. \tag{1.41}$$

(iv) The entropy as a function of (T, V) *is given by*

$$S(T,V) = nR\ln\frac{V}{V_r} + \int_{T_r}^{T}\frac{C_V(\tau)}{\tau}\,\mathrm{d}\tau + S_r. \tag{1.42}$$

---

[16] $[m_A] = \mathrm{kg}$

Proof: Considering $E = E(S(T,V),V)$ we obtain the useful relation

$$\left(\frac{\partial E}{\partial V}\right)_T = \left(\frac{\partial E}{\partial S}\right)_V \left(\frac{\partial S}{\partial V}\right)_T + \left(\frac{\partial E}{\partial V}\right)_S \overset{(1.20)}{=} T\left(\frac{\partial p}{\partial T}\right)_V - p. \tag{1.43}$$

Obviously this is zero for the ideal gas EOS. Using Lemma 1.3.2 (i) then gives $C_V = C_V(T)$ and thus together we have (iii). Further we use Lemma 1.3.2 (iii) and yield

$$C_p - C_V = \frac{\alpha^2 VT}{\kappa_T} = \frac{PV}{T} = nR.$$

Hence this immediately results in $C_p = C_p(T)$. For the entropy we use

$$\left(\frac{\partial S}{\partial T}\right)_V = \frac{C_V(T)}{T} \quad \text{and} \quad \left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial p}{\partial T}\right)_V.$$

Integrating from a reference temperature T_r to T and from a reference volume V_r to V respectively gives the desired result. □

An explicit relation for $C_V(T)$ would complete the picture and we could calculate the caloric EOS. If we assume the heat capacities to be constant we conclude [17]

$$E(T) = C_V(T - T_r) + E_r, \tag{1.44}$$
$$S(T,V) = nR \ln\frac{V}{V_r} + C_V \ln\frac{T}{T_r} + S_r. \tag{1.45}$$

---

[17] In this case one may find different names for this kind of EOS, such as *perfect*, *simple* or *polytropic* gas EOS. It is also quite common to even use the name ideal gas EOS in both situations

Hence the Gibbs energy for a perfect gas is given by (using (1.13))

$$\begin{aligned}
V(T,p) &= \frac{nRT}{p},\\
S(T,V(T,p)) &= nR\ln\left(\frac{p_r}{p}\frac{T}{T_r}\right) + C_V\ln\frac{T}{T_r} + S_r,\\
G(T,p) &= E(T,p) - TS(T,p) + pV(T,p),\\
&= C_V(T-T_r) + E_r - T\left(nR\ln\frac{p_r}{p} + (C_V+nR)\ln\frac{T}{T_r} + S_r\right) + nRT,\\
&= nRT\ln\frac{p}{p_r} + (C_V+nR)\left(T - T_r - T\ln\frac{T}{T_r}\right) - (T-T_r)S_r + G_r,
\end{aligned} \tag{1.46}$$

$$G_r := E_r - T_rS_r + p_rV_r.$$

If we now consider an isothermal process at some fixed temperature T^* and choose $T_r = T^*$ we immediately obtain

$$G(T_r,p) = nRT_r\ln\frac{p}{p_r} + G_r. \tag{1.47}$$

In a similar way one may obtain every other potential. For later use we want to give the dimensionless quantities and the sound speed for the ideal gas.

Proposition 1.3.9. *Given the ideal gas EOS (1.39) and a caloric EOS (yet to be specified). The quantities defined in 1.3.3 are given by*

$$\begin{aligned}
&\gamma = 1 + \frac{nR}{C_V(T)},\ g = \gamma - 1,\ \Gamma = \gamma - 1,\ \mathcal{G} = \frac{1}{2}(\gamma+1) + \frac{1}{2}\frac{\gamma-1}{\gamma}\frac{\mathrm{d}\gamma}{\mathrm{d}T},\\
&\gamma_T = 1 \quad \textit{and} \quad \mathcal{G}_T = 1.
\end{aligned}$$

For the sound speed one obtains using the results of Lemma 1.3.7

$$\begin{aligned}
a^2 &= a^2(T) = \gamma nRT,\\
a_T^2 &= nRT,\ T = \textit{const}.
\end{aligned}$$

Proof: We omit the details of this proof, since it is just a combination of Definitions 1.3.1, 1.3.3 and of the thermodynamic identities derived before.

□

Note that in the case of an ideal gas γ is the adiabatic exponent as usually defined with $\gamma = C_P/C_V$ and may depend on the temperature. However, for other EOS this is in general not true and instead the following relation holds due to Lemma 1.3.2 (iii), see [60]

$$\frac{C_p}{C_V} = \frac{\gamma g}{\gamma g - \Gamma^2}. \tag{1.48}$$

Regarding the convexity of E (see (1.31)), one verifies that this holds for $\gamma \geq 1$ and strict convexity for $\gamma > 1$. This finishes our discussion of the ideal gas.

Another EOS often used for fluid flow problems, especially when liquids are considered, is the *stiffened gas* or *Tammann* EOS [18]. In terms of (E, V) it reads

$$\begin{aligned} p(E, V) &= (\gamma_0 - 1)\frac{E - E_\infty}{V} - \gamma_0 p_\infty, \\ p_r &= p(E_r, V_r). \end{aligned} \tag{1.49}$$

For a detailed discussion see [60], Flåtten et al. [33] and Saurel et al. [73]. We want to calculate the entropy and the temperature under the assumption of constant heat capacities. Once obtained, other potentials may be derived using the adequate formulas derived before. It is easy to see, that for $p_\infty = 0$ and $E_\infty = 0$ (1.49) reduces to the ideal gas EOS.

Proposition 1.3.10. *For the stiffened gas EOS (1.49) the entropy and temperature are given by*

$$\begin{aligned} S(p, V) &= C_p \ln\left(\frac{V}{V_r}\left(\frac{p + p_\infty}{p_r + p_\infty}\right)^{\frac{1}{\gamma_0}}\right) \overset{C_p = \gamma_0 C_V}{=} C_V \ln\left(\left(\frac{V}{V_r}\right)^{\gamma_0} \frac{p + p_\infty}{p_r + p_\infty}\right) \\ T(p, V) &= \frac{\gamma_0 (p + p_\infty) V}{C_p(\gamma_0 - 1)} \overset{C_p = \gamma_0 C_V}{=} \frac{(p + p_\infty) V}{C_V(\gamma_0 - 1)}. \end{aligned}$$

---

[18] It is remarked in [60] that the stiffened gas EOS can be seen as an approximation of any EOS near a reference state (E_r, V_r) with quadratic errors in $V - V_r$ and $E - E_r$.

Further the dimensionless quantities are

$$\gamma = \gamma_0 \left(1 + \frac{p_\infty}{p}\right),\ g = (\gamma_0 - 1)\frac{p}{p + p_\infty},\ \Gamma = \gamma_0 - 1,\ \mathcal{G} = \frac{1}{2}(\gamma_0 + 1),$$
$$\gamma_T = 1 + \frac{p_\infty}{p} \quad \textit{and} \quad \mathcal{G}_T = 1.$$

According to the results of Lemma 1.3.7 the sound speeds are given by

$$a^2 = a^2(T) = \gamma_0 v(p + p_\infty) = \gamma_0(\gamma_0 - 1)c_v T,$$
$$a_T^2 = c_v(\gamma_0 - 1)T,\ T = const.$$

Proof: We want to derive the relations in terms of the volume V and the pressure p. The state space is denoted by $\Omega \subset \mathbb{R}^2$. We obtain for the differential of the internal energy E using (1.49)

$$\mathrm{d}E = \left(\frac{\partial E}{\partial p}\right)_V \mathrm{d}p + \left(\frac{\partial E}{\partial V}\right)_p \mathrm{d}V = \frac{V}{\gamma_0 - 1}\mathrm{d}p + \frac{p + \gamma_0 p_\infty}{\gamma_0 - 1}\mathrm{d}V.$$

Using (1.5) we obtain for the entropy

$$\mathrm{d}S = \frac{1}{T}\mathrm{d}E + \frac{p}{T}\mathrm{d}V = \frac{V}{(\gamma_0 - 1)T}\mathrm{d}p + \frac{1}{T}\left(\frac{p + \gamma_0 p_\infty}{\gamma_0 - 1} + p\right)\mathrm{d}V.$$

Hence we have two equations for the temperature

$$\frac{1}{T} = \frac{\gamma_0 - 1}{V}\left(\frac{\partial S}{\partial p}\right)_V \quad \text{and} \quad \frac{1}{T} = \frac{\gamma_0 - 1}{\gamma_0 (p + p_\infty)}\left(\frac{\partial S}{\partial V}\right)_p.$$

Equalizing these two equations for T gives a hyperbolic *PDE* for the entropy S

$$V\left(\frac{\partial S}{\partial V}\right)_p - \gamma_0(p + p_\infty)\left(\frac{\partial S}{\partial p}\right)_V = 0.$$

Once the entropy is determined, we are able to calculate all remaining quantities. We assume the following relation between entropy and volume [19]

$$S \sim C \ln \frac{V}{V_r}.$$

---

[19] This can be justified by thermodynamical as well as statistical considerations. Nevertheless more general choices are possible, see [60]

Now we can write down the full problem (with a fixed p_r)

$$\begin{cases} V\left(\dfrac{\partial S}{\partial V}\right)_p - \gamma_0(p+p_\infty)\left(\dfrac{\partial S}{\partial p}\right)_V & = 0,\ (p,V)\in\Omega, \\ S(p_r,V) & = C_p \ln \dfrac{V}{V_r},\ (p_r,V)\in\Omega. \end{cases}$$

This *PDE* can be solved by the *Method of Characteristics* (see Evans [28]) which transforms it into a system of *ODEs* for σ

$$\begin{cases} \dot{x}_1(\sigma,\xi) & = \gamma_0(x_1+p_\infty),\ x_1(0,\xi) = p_r, \\ \dot{x}_2(\sigma,\xi) & = x_2,\ x_2(0,\xi) = \xi, \\ \dot{z}(\sigma,\xi) & = 0,\ z(0,\xi) = C_p \ln \frac{\xi}{V_r}. \end{cases}$$

We yield the following solution

$$\begin{aligned} x_1(\sigma,\xi) &= (p_r+p_\infty)e^{\gamma_0\sigma} - p_\infty, \\ x_2(\sigma,\xi) &= \xi e^{\sigma}, \\ z(\sigma,\xi) &= C_p \ln \frac{\xi}{V_r}. \end{aligned}$$

Expressed in (x_1,x_2) we have

$$\begin{aligned} \sigma(x_1) &= \frac{1}{\gamma_0}\ln\frac{x_1+p_\infty}{p_r+p_\infty}, \\ \xi(x_1,x_2) &= x_2\left(\frac{x_1+p_\infty}{p_r+p_\infty}\right)^{-\frac{1}{\gamma_0}}, \\ z(x_1,x_2) &= C_p \ln\left(\frac{x_2}{V_r}\left(\frac{x_1+p_\infty}{p_r+p_\infty}\right)^{\frac{1}{\gamma_0}}\right). \end{aligned}$$

So we obtain for the entropy and temperature

$$\begin{aligned} S(p,V) &= C_p \ln\left(\frac{V}{V_r}\left(\frac{p+p_\infty}{p_r+p_\infty}\right)^{\frac{1}{\gamma_0}}\right) \overset{C_p=\gamma_0 C_V}{=} C_V \ln\left(\left(\frac{V}{V_r}\right)^{\gamma_0}\frac{p+p_\infty}{p_r+p_\infty}\right) \\ T(p,V) &= \frac{\gamma_0(p+p_\infty)V}{C_p(\gamma_0-1)} \overset{C_p=\gamma_0 C_V}{=} \frac{(p+p_\infty)V}{C_V(\gamma_0-1)}. \end{aligned}$$

The dimensionless quantities and sound speeds are obtained as before. □

One verifies that these equation reduce to the ones for the ideal gas if we choose $E_\infty = 0$ and $p_\infty = 0$. Note that for the stiffened gas EOS the quotient of the heat capacities and the adiabatic exponent are not equal, i.e. $C_P/C_V = \gamma_0 \neq \gamma$. Regarding thermodynamic stability it is clear that $p \geq 0$ [20] and thus with $p_\infty \geq 0$ we have $\gamma \geq \gamma_0$. For $g \geq 0$ we require $\gamma_0 \geq 1$ and then $\gamma g \geq \Gamma^2$ follows immediately.

1.3.2 Linear and Non-Linear Tait EOS

In this section we want to present the linear and the non-linear *Tait EOS* and derive the corresponding quantities such as entropy and internal energy. Therefore we will use the established thermodynamic relations in order to obtain a consistent formulation. The isothermal *Tait EOS*

$$p(V) = p_r + K_r\left(\left(\frac{V_r}{V}\right)^\nu - 1\right) \tag{1.50}$$

is for example discussed and used in [23, 25, 37, 46, 72]. Quantities with subscript r are constant reference values at a given temperature T_r. Here K_r is the modulus of compression ($[K_r] = \text{Pa}$). The non-linearity is due to the exponent $\nu \geq 1$ and we refer to the *linear Tait EOS* for $\nu = 1$. In [23, 37] the linear Tait EOS is used and the reference constants p_r, K_r and V_r were chosen at the saturation state for a given temperature T_r according to [84]. The non-linear Tait EOS is for example used in [46] and [72]. In particular, it was shown in [46] that the equation for the energy balance (2.65) decouples from (2.63) and (2.64) if one uses (1.50). This is not surprising, because the full Euler system is temperature dependent.

Here we want to derive the relations for a temperature dependent Tait EOS. The isothermal case is then easily obtained by fixing T. The main idea is to replace the (temperature dependent) constants in (1.50) by temperature dependent functions. In fact also the exponent is weakly temperature dependent, but this is neglected here. A similar idea was proposed in [72] but the corresponding internal energy is not calculated. Instead the internal

---

[20] In general negative pressures are possible in liquids, see Davitt et al. [19]. Nevertheless a system with negative pressure is not thermodynamic stable and thus the internal energy is not convex anymore. However one can still use (1.49) but has to be very careful with interpreting the results.

energy for the isothermal case is presented. The temperature dependent *Tait EOS* reads

$$p(V,T) = \bar{p}(T) + \bar{K}(T)\left(\left(\frac{\bar{V}(T)}{V}\right)^{\nu} - 1\right). \tag{1.51}$$

We want to emphasize that the functions $\bar{p}, \bar{K}$ and $\bar{V}$ do not necessarily have to represent actual physical quantities. They represent general temperature dependent functions which will be specified later on and of course should ensure thermodynamic stability.

Proposition 1.3.11 (Linear Tait EOS)**.** *Consider the Tait EOS (1.51) with $\nu \geq 1$, then the internal energy and entropy are given as follows*

$$\begin{aligned} E(V,T) &= A(T)\,(V - V_r) + B(T)\Phi(V) + \int_{T_r}^{T} C_V(V_r,\tau)\,\mathrm{d}\tau + E_r, \\ S(V,T) &= \bar{A}(T)\,(V - V_r) + \bar{B}(T)\Phi(V) + \int_{T_r}^{T} \frac{C_V(V_r,\tau)}{\tau}\,\mathrm{d}\tau + S_r \end{aligned}$$

with

$$\begin{aligned} C_V(V,T) &= A'(T)(V - V_r) + B'(T)\Phi(V) + C_V(V_r,T), \\ \bar{A}(T) &= \bar{p}'(T) - \bar{K}'(T), \\ \bar{B}(T) &= -\frac{\mathrm{d}}{\mathrm{d}T}\left(\bar{K}(T)\bar{V}(T)^{\nu}\right), \\ A(T) &= T\bar{A}(T) - \left(\bar{p}(T) - \bar{K}(T)\right), \\ B(T) &= T\bar{B}(T) + \bar{K}(T)\bar{V}(T)^{\nu}, \\ \Phi(V) &= \begin{cases} \ln\dfrac{V_r}{V}, \ \nu = 1 \\ \dfrac{1}{1-\nu}\left(\dfrac{1}{V^{\nu-1}} - \dfrac{1}{V_r^{\nu-1}}\right), \ \nu > 1 \end{cases}. \end{aligned}$$

The prime denotes the derivative with respect to T. The dimensionless quantities *are given by* [21]

$$\gamma = \nu\frac{\bar{K}(T)\bar{V}(T)^\nu}{pV^\nu} + \frac{\Gamma^2}{g},\ g = \frac{pV}{TC_V},\ \Gamma = \frac{V}{C_V}\left(\bar{A}(T) - \frac{\bar{B}(T)}{V^\nu}\right),$$
$$\gamma_T = \nu\frac{K_r V_r^\nu}{pV^\nu} \quad \text{and} \quad \mathcal{G}_T = \frac{\nu+1}{2}.$$

The sound speeds are according to Lemma 1.3.7

$$a^2 = \gamma p V,$$
$$a_T^2 = \nu\frac{K_r V_r^\nu}{V^{\nu-1}}.$$

Proof: In order to derive the internal energy $E(V,T)$ we use Lemma 1.3.2 (i) and (1.43)

$$(a)\ \left(\frac{\partial E}{\partial T}\right)_V = C_V(V,T), \quad (b)\ \left(\frac{\partial E}{\partial V}\right)_T = T\left(\frac{\partial p}{\partial T}\right)_V - p.$$

From these relations we obtain the internal energy by integration with respect to T and V. Analogously we obtain the entropy using 1.3.1 (i) and (1.20)

$$(a)\ \left(\frac{\partial S}{\partial T}\right)_V = \frac{C_V(V,T)}{T}, \quad (b)\ \left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial p}{\partial T}\right)_V.$$

The remaining quantities are obtained as before. □

Remark 1.3.12. *We want to comment on the above results.*

(i) Considering (1.50) with $\nu = 1$ and $C_V(V_r,T) = C_V = const.$ we obtain

$$E(V,T) = (K_r - p_r)(V - V_r) + K_r V_r \ln\frac{V_r}{V} + C_V(T - T_r) + E_r,$$
$$S(V,T) = S(T) = C_V \ln\frac{T}{T_r} + S_r.$$

---

[21] In this case we omit the calculation of $\mathcal{G}$, due to the complexity of formula (1.34) and the rather general assumptions on the EOS. However, regarding [76] the Tait EOS with $\nu = 7$ seems to be a good fit for liquid water concerning the fundamental derivative.

These are exactly the expressions obtained in [23]. Note that the entropy for (1.50) does not depend on the density, as remarked in [23]. This due to the fact that the derivatives of $\bar{p}(T)$, $\bar{K}(T)$ *and* $\bar{V}(T)$ *at* $T = T_r$ *are neglected here. Beware of the difference between first choosing these functions constant and after that calculate the entropy etc. or first calculate all quantities and then chooses* $T = const.$.

(ii) *In [46] Ivings et al. used the Tait EOS (1.50) without* p_r. *Note that for (1.50) one obtains* $\Gamma = 0$ *according Proposition 1.3.11. Thus we have for the ratio of the heat capacities, according to (1.48),* $C_p/C_V = 1$. *This is independent of the choice of* $\nu \geq 1$ *and* $C_V(V_r, T)$.

(iii) *As mentioned before, Saurel et al. proposed to choose* $\bar{p}(T)$ *and* $\bar{V}(T)$ *to be the values at the saturation line for liquid water, see [72].* $\bar{K}(T)$ *is assumed to be constant* K_r *and further they used* $\nu = 7$. *In this case the isochoric heat capacity* will not *be constant.*

(iv) *So far we have not specified the caloric EOS, but in view of the determined equations it is sufficient to know* $C_V(V_r, T)$. *In fact, one can write (compare [5])*

$$C_V(V,T) = C_V(V_r,T) + T\int_{V_r}^{V}\left(\frac{\partial^2 p}{\partial T^2}\right)_V(\sigma,T)\,\mathrm{d}\sigma.$$

(v) *Concerning the convexity of* $E(V,S)$ *we again recall (1.31). Up to now* $C_V(V,T)$ *is not specified completely (a possible choice still could be* $C_V = const.$*), however it must satisfy* $C_V > 0$. *Further we require* $\bar{K}(T)\bar{V}(T)^\nu > 0$. *The positivity of* p, V *and* T *of course is mandatory. With this at hand it follows that* $\gamma g \geq \Gamma^2$ *and thus the convexity of* E.

(vi) *Note that the linear Tait EOS (1.51) is equivalent to the stiffened gas EOS (1.49) for the following particular choice*

$$\bar{p}(T) - \bar{K}(T) = -p_\infty \quad \textit{and} \quad \bar{K}(T)\bar{V}(T) = C_V(\gamma_0 - 1)T.$$

Therefore both are sometimes called Tammann EOS, see [33] and [46].

1.4 Thermodynamics for Multiphase Systems

In this section we briefly want to give some results for thermodynamic systems containing multiple phases. Generally by *phase* one denotes a *chemically* and a *physically* homogeneous part of a thermodynamic system. Chemically different substances in a system are called components. If only one component is considered the different aggregate states, e.g. solid, liquid and vapor, are also called phases. In this work we only want to consider systems with one component (e.g. water) and two phases, i.e. liquid and vapor phases.

Let the thermodynamic system be completely described by the entropy S, the volume V and the mole number N. Hence in view of (1.4) we have for the internal energy and entropy

$$\mathrm{d}E = T\mathrm{d}S - p\mathrm{d}V + \mu\mathrm{d}N, \tag{1.52}$$

$$\mathrm{d}S = \frac{1}{T}\mathrm{d}E + \frac{p}{T}\mathrm{d}V - \frac{\mu}{T}\mathrm{d}N. \tag{1.53}$$

The other potentials can be extended accordingly. The chemical potential μ quantifies the change of the internal energy when particles are added or removed from the system. Now consider an isolated system of two phases, each described by (E_i, V_i, N_i), $i = 1, 2$, see [5]. For the whole system the quantities (E, V, N) are kept constant and thus the partial quantities are not independent from each other, i.e.

$$E_2 = E - E_1,\ V_2 = V - V_1 \text{ and } N_2 = N - N_1.$$

Further two phases in an isolated system are in equilibrium when the entropy is maximized and thus we get

$$0 = \mathrm{d}S = \mathrm{d}S_1 + \mathrm{d}S_2 = \left(\frac{1}{T_1} - \frac{1}{T_2}\right)\mathrm{d}E_1 + \left(\frac{p_1}{T_1} - \frac{p_2}{T_2}\right)\mathrm{d}V_1 + \left(\frac{\mu_1}{T_1} - \frac{\mu_2}{T_2}\right)\mathrm{d}N_1.$$

Since the internal energy, volume and mole number of phase one may change arbitrarily, we obtain the equilibrium conditions for the case of a one component system with two phases

$$T_1 = T_2,\ p_1 = p_2,\ \mu_1 = \mu_2. \tag{1.54}$$

The conditions describe *thermal* (T), *mechanical* (p) and *phase* equilibrium (μ). Considering (1.54) we express the potential in terms of (T, p) and obtain

$$\mu_1(T, p) = \mu_2(T, p). \tag{1.55}$$

This equation directly shows that a two phase equilibrium is not possible for arbitrary combinations of temperature and pressure. Conversely (1.55) defines a curve in the $T-p$ plane. Such a curve separates homogeneous phases

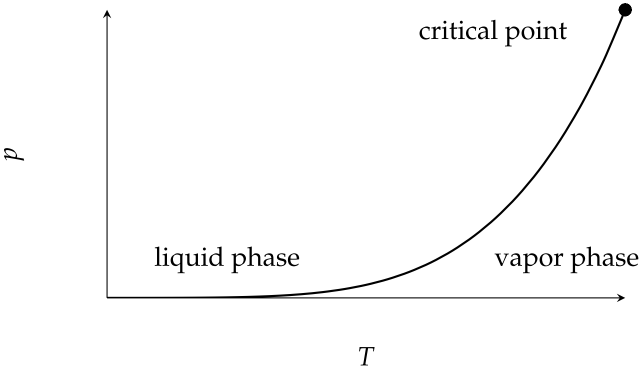

Figure 1.1: Saturation curve in the $T - p$ plane

of a substance and is often called *coexistence curve* or *saturation boundary*, see Figure 1.1. Across this curve the Gibbs energy suffers jumps in its first order derivatives. This gives rise to the *Ehrenfest classification* of phase transitions, where the order of the phase transition is given by the order of the lowest derivative of G that is discontinuous. Hence liquid–vapor phase transitions below the critical point are first order phase transitions with discontinuities in (see (1.17))

$$\left(\frac{\partial G}{\partial T}\right)_p = -S \quad \text{and} \quad \left(\frac{\partial G}{\partial p}\right)_T = V.$$

Due to the Gibbs–Duhem relation (1.18) we obtain

$$\mathrm{d}\mu = \frac{\mathrm{d}G - \mu \mathrm{d}N}{N} = v\mathrm{d}p - s\mathrm{d}T. \tag{1.56}$$

Where v and s are specific quantities per particle. Now using (1.55) gives

$$\mathrm{d}\mu_1 = \mathrm{d}\mu_2 \quad \Leftrightarrow \quad v_1\mathrm{d}p - s_1\mathrm{d}T = v_2\mathrm{d}p - s_2\mathrm{d}T$$

and hence we obtain the *Clausius–Clapeyron* equation

$$\frac{\mathrm{d}p}{\mathrm{d}T} = \frac{s_2 - s_1}{v_2 - v_1} = \frac{\Delta q}{T\Delta v}. \tag{1.57}$$

Here $\Delta q = T\Delta s$ is the latent heat per particle, see [51, 70]. Equation (1.57) determines the slope of the coexistence curve in the $T - p$ plane. All points on this coexistence curve represent states where phase equilibrium states are possible.

Due to the discontinuity of the volume the situation changes if the $V - T$ plane is considered instead. Now these states fill a whole domain in the plane. Left and right to this domain are the homogeneous phases and inside the domain are mixed states of the adjacent phases. Note that for a pure state the inequalities (1.31) are strict whereas a point in the mixed phase region may be written as

$$v = (1-\alpha)v_1 + \alpha v_2,\ s = (1-\alpha)s_1 + \alpha s_2 \text{ and } e = (1-\alpha)e_1 + \alpha e_2 \text{ for } \alpha \in (0,1).$$

Hence the (specific) internal energy is not strict convex anymore, i.e. $\gamma g = \Gamma^2$. Further all states given by the equations above are mapped onto the same values of p, T and g by the Legendre transform, see [60].

The coexistence curve ends in a single point which is called the *critical point*. Quantities at the critical point are also called critical. There exist no distinct phases for temperatures above T_c or pressures above p_c. In particular the entropy and the specific volume become continuous. A consequence is, that above the critical point only phase transitions of second order are possible. It is shown in [51] that there exists a curve inside the mixed phase region that separates the whole domain where the thermodynamic inequalities fail to be true. This curve can be found by investigating

$$\left(\frac{\partial p}{\partial V}\right)_T = 0.$$

In points where this derivative vanishes the isotherms end, due to the violation of $\gamma_T > 0$. Further this curve is often referred to as *spinodal* curve or line, e.g. [59]. The enclosed interior region is called *spinodal region*, see Figure 1.2. For an exemplary discussion of the spinodal of liquid water see Poole et al. [69]. Given the equilibrium condition (1.54) it follows that points on the coexistence curve with equal temperature in the $v - T$ plane are connected by horizontal straight lines. The same holds for the $v - p$ plane respectively. There are no conditions, given which it is possible that a substance exists in a homogeneous state inside this domain. However the states between the spinodal curve and the coexistence curve are so called *meta stable* states. When in a meta stable state, the substance is in a homogeneous phase although it should have changed its state when in complete equilibrium. Depending on the phase these states are called *overheated liquid* or *undercooled vapor*. Usually a small disturbance of such

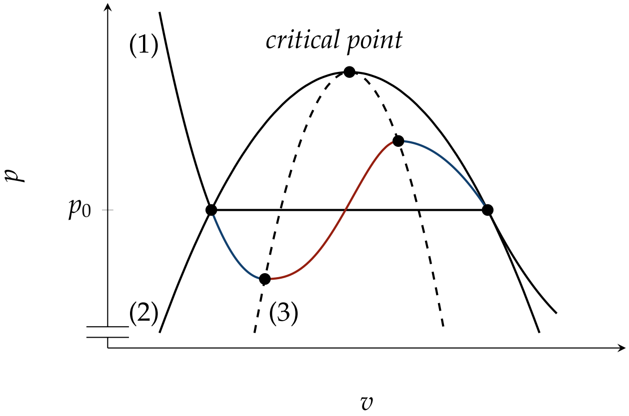

Figure 1.2: Schematic figure of the $v - p$ phase plane. Curve (1) is an isotherm with $T = T_0$. Curve (2) is the saturation boundary with the liquid on the outer left side and the vapor on the outer right side, respectively. Curve (3) is the spinodal curve. The region between curve (2) and curve (3) is the metastable region whereas the area enclosed by curve (3) is the spinodal region. The blue parts of the isotherm are the metastable states and the horizontal black line is the coexistence curve in the $v - p$ plane.

a system will immediately lead to a phase transition. According to [65] it is possible to compress vapor up to a pressure p *four times* larger than the corresponding saturation pressure without condensation. The above results are most often visualized using the *van-der-Waals* equation of state

$$nRT = \left(p + \frac{an^2}{V^2}\right)(V - nb)\,. \tag{1.58}$$

The van-der-Waals EOS is obtained by taking the size of the particles and their interactions into account. Since we do not want to focus on this particular EOS see [5, 58, 47] for details. Isotherms of a van-der-Waals fluid for temperatures below the critical temperature T_c exhibit two extremal points enclosing an interval where

$$\left(\frac{\partial p}{\partial V}\right)_T > 0.$$

States inside this interval do not correspond to any realizable homogeneous state in nature, see [51].

As mentioned before, a equilibrium transition between a liquid and vapor state is a horizontal straight line. This line can be found using (1.55). We have along an isotherm

$$0 = \int_1^2 \mathrm{d}\mu \overset{(1.56)}{=} \int_1^2 v\,\mathrm{d}p. \tag{1.59}$$

This formula states that the two areas enclosed by the isotherm and the horizontal line must be equal. Therefore it is often called *equal–area–rule*. Quite often it is also referred to as *Maxwell construction*. When expressed in terms of the volume one yields at T_0

$$0 = p_0(T_0)(v_2 - v_1) - \int_{v_1}^{v_2} p(v, T_0)\,\mathrm{d}v. \tag{1.60}$$

Then the areas between the isobar at pressure $p_0(T_0)$ and the isotherm at temperature T_0 are equal, see Figure 1.2.
Another point of view concerning the Maxwell construction might be as follows. Assume we connect an EOS for the liquid state and one for the vapor state continuously at the fixed temperature T_0. Let us further prescribe the pressure $p_0(T_0)$ and the *minimum liquid pressure* p_{min} (e.g. $p_{min} = 0$). Now we may calculate the maximum vapor pressure $\tilde{p}$ using the Maxwell construction (1.60) as follows, see also Figure 1.3.

Definition 1.4.1 (Maximum Vapor Pressure)**.** *Given a fixed temperature T_0 the corresponding saturation pressure p_0 is given by (1.55). Furthermore p_{min} is defined to be the minimum liquid pressure. Let $\bar{v}(p)$ be a function such that*

$$v_L(p_{min}) = \bar{v}(p_{min}), \quad v_V(\tilde{p}) = \bar{v}(\tilde{p}) \quad \textit{and} \quad \bar{v}'(p) > 0.$$

Then the maximum vapor pressure $\tilde{p}$ is found as the solution of the following equation

$$0 = p_0(v_V(p_0) - v_L(p_0)) - \int_{v_L(p_0)}^{v_V(p_0)} p(v)\,\mathrm{d}v.$$

The function $p(v)$ given by

$$p(v) = \begin{cases} p_L(v), \; v \in (0, v_L(p_{min})] \\ \bar{p}(v), \; v \in (v_L(p_{min}), v_V(\tilde{p})), \\ p_V(v), \; v \in [v_V(\tilde{p}), \infty) \end{cases} .$$

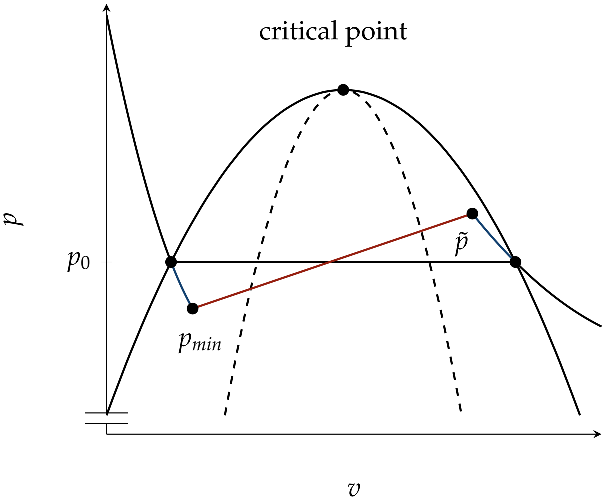

Figure 1.3: Schematic figure of the $v-p$ phase plane with the Maxwell construction for the case considered in Definition 1.4.1.

1.4.1 Thermodynamics of a Surface

In the presence of two phases one has to consider effects related to the presence of the surface separating the two phases. Therefore we briefly want to present some results related to a surface. The presented results can be found in the following works [7, 21, 35, 36, 52, 64, 65] and [80].

To this end we follow [21] and [52]. Let us consider a surface $\mathcal{S}$ with a total area A ($[A] = \mathrm{m}^2$). In a reversible process the work needed to change A by the infinitesimal amount dA is directly proportional to dA, i.e.

$$\mathrm{d}W = \sigma \mathrm{d}A. \tag{1.61}$$

The quantity σ is called *coefficient of the surface tension* or sometimes, quite misleading, just *surface tension* and is a force per line ($[\sigma] = \mathrm{N/m}$). It is a fundamental surface quantity which is strictly positive, otherwise different phases could not exist, see [52].

If we consider two phases of a single substance at constant temperature the work in (1.61) is equal to the change of the surface free energy

$$\mathrm{d}F_{\mathcal{S}} = \sigma \mathrm{d}A. \tag{1.62}$$

Let $T_{\mathcal{S}}$ and $S_{\mathcal{S}}$ denote the surface temperature and the surface entropy, respectively. If we assume that the surface free energy is related to the surface entropy in the usual way (see (1.14)) we may write

$$\mathrm{d}F_{\mathcal{S}} = -S_{\mathcal{S}}\mathrm{d}T_{\mathcal{S}} + \sigma \mathrm{d}A. \tag{1.63}$$

In complete analogy to (1.15) and (1.20) we obtain the following relations

$$S_{\mathcal{S}} = -\left(\frac{\partial F_{\mathcal{S}}}{\partial T_{\mathcal{S}}}\right)_A, \quad \sigma = \left(\frac{\partial F_{\mathcal{S}}}{\partial A}\right)_{T_{\mathcal{S}}} \quad \text{and} \quad \left(\frac{\partial S_{\mathcal{S}}}{\partial A}\right)_{T_{\mathcal{S}}} = \left(\frac{\partial \sigma}{\partial T_{\mathcal{S}}}\right)_A. \tag{1.64}$$

If we consider a small surface element A with a uniform temperature we may assume that there are densities per unit area such that we have

$$F_{\mathcal{S}} = f_{\mathcal{S}}(T_{\mathcal{S}})A \quad \text{and} \quad S_{\mathcal{S}} = s_{\mathcal{S}}(T_{\mathcal{S}})A. \tag{1.65}$$

Thus we conclude using (1.62) and (1.63)

$$f_{\mathcal{S}} = \sigma \quad \text{and} \quad s_{\mathcal{S}} = -\frac{\mathrm{d}\sigma}{\mathrm{d}T_{\mathcal{S}}}. \tag{1.66}$$

Hence the coefficient of the surface tension is also called *surface free energy density*. This result may also be found in the works of Gurtin [35, 36]. A direct consequence can be obtained for the internal surface energy $e_{\mathcal{S}}$, i.e.

$$\begin{aligned} &\sigma \overset{(1.66)_1}{=} f_{\mathcal{S}} \overset{(1.11)}{=} e_{\mathcal{S}} - T_{\mathcal{S}}s_{\mathcal{S}} \\ &\Leftrightarrow \\ &e_{\mathcal{S}} = \sigma + T_{\mathcal{S}}s_{\mathcal{S}} \overset{(1.66)_2}{=} \sigma - T_{\mathcal{S}}\frac{\mathrm{d}\sigma}{\mathrm{d}T_{\mathcal{S}}} = -T_{\mathcal{S}}^2\frac{\mathrm{d}}{\mathrm{d}T_{\mathcal{S}}}\left(\frac{\sigma}{T_{\mathcal{S}}}\right). \end{aligned} \tag{1.67}$$

This formula can be found in [52] or in another context for example in [11]. Without derivation we want to cite a relation between the σ and the temperature as given in [52] (§154, p. 494). The relation is given by

$$\sigma \sim (T_c - T)^{2\nu}. \tag{1.68}$$

Here T_c is the critical temperature and $2\nu \approx 1.3$.

In general the coefficient of the surface tension can depend on much more quantities than just the surface temperature, see [21] and [36]. For example the geometry of the surface might be respected through the dependence on the surface normal. Nevertheless it is shown in these works that certain conditions need to hold to ensure compatibility with thermodynamics. In particular the equations (1.66) need to hold for the more general cases. We will not discuss this in detail and refer to the afore mentioned literature.

2 Concepts: Balance Laws

In the present chapter we want to introduce the laws used to describe the dynamics of the fluid motion. These laws are in general referred to as *balance laws*. The key contribution from physics to this topic is provided by the theory for irreversible processes and nonequilibrium thermodynamics. Results for nonequilibrium thermodynamics can be found in the works of Bedeaux [7], Mauri [59] and DeGroot and Mazur [20]. Here we want to focus more on the physical/modeling aspects of the balance laws rather than the mathematical theory. We assume that the reader is familiar with most of the mathematical concepts in this field.

An introduction to balance laws from a thermodynamic point of view can be found in Landau et al. [52], Müller [64] and Müller & Müller [65]. In Section 2.1 we will present a general derivation of balance laws as it can be found in [21] and [64]. A further derivation of balance laws in the presence of interfaces may be found in Bedeaux [7]. A treatment of this topic in two dimensions can be found in the book of Gurtin [36].

The main part of this work uses the Euler equations and therefore we will focus on them. In particular the Euler equations are special balance laws, precisely they are a system of conservation laws. Conservation laws describe the dynamics of a fluid under the constraint that certain physical quantities are conserved, i.e. there total change in time is zero. The field of conservation laws, even when restricted to particular equations, is far to extensive to be pictured here. A derivation of particular conservation laws based on the results of Section 2.1 is therefore given in Section 2.2.

A brief overview of the mathematical results for *hyperbolic partial differential equations*, in particular *hyperbolic conservation laws*, is given in Section 2.3. In this context we, without being complete, refer to the following literature. The book on partial differential equations by Evans [28] contains a compact

description of the topic, especially of systems of conservation laws. An exhaustive introduction and discussion of analytical methods for conservation laws can be found in the book of Warnecke [85]. Further we recommend the books by Dafermos [18], LeFloch [55] and Smoller [75]. The books [18, 55] give a precise treatment of hyperbolic conservation laws. Especially [18] starts with a very general approach, introducing the balance laws in terms of suited measures and further gives a nice historical review of the topic. The book [75] does not focus on hyperbolic conservation laws alone, but it also treats reaction-diffusion equations. For additional literature see the references in the previous mentioned literature.
As mentioned before we focus on the Euler equations. Therefore we will introduce them in Section 2.4 with respect to the previous sections.

2.1 Generic Balance Laws

In this section we want to derive generic equations that for example may be used to describe the dynamics of a fluid in the presence of interfaces. These equations are referred to as *balance laws*. To be more precise we want to derive the local description of a general balance law in three dimensions. This will allows us to derive several relations from one general equation, highlighting the deep connection between all the resulting equations. We will present a general derivation as it can be found in [21] and [64]. Therefore we also recommend the works of Aris [2] and Truesdell and Toupin [79] [1]. For the treatment of moving surfaces in three dimensions we refer to the suited literature such as the book of Grinfeld [34]. A further derivation of balance laws in the presence of interfaces may be found in Bedeaux [7]. Although the resulting equations are not needed in their entire generality, we want to follow this approach. Here the main benefit is that the effects of simplifying assumptions may be emphasized properly. Thus one immediately can see the arising difficulties if certain assumptions are dropped.

Let $\mathcal{V}(t) \subset \mathbb{R}^3$ be a time dependent material volume, i.e. there is no mass flux through the boundary $\partial\mathcal{V}(t)$ of $\mathcal{V}(t)$. Thus the boundary moves with

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[1] Reference [79] is also very interesting from a historical perspective of view, since it presents the results in the context of original works. Thus the influences of mathematicians like *Christoffel, Euler, Hadamard, Hugoniot, Reynolds* on this topic become apparent.

the velocity of the particles included in $\mathcal{V}(t)$ [2]. Further let $\mathcal{S}(t)$ be the surface separating $\mathcal{V}$ into two regions denoted by $\mathcal{V}_1(t)$ and $\mathcal{V}_2(t)$. Such a situation is sketched in Figure 2.1.

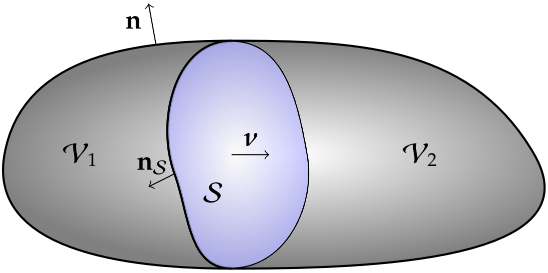

Figure 2.1: An arbitrary material volume $\mathcal{V}$ separated by an internal surface $\mathcal{S}$. The sub-volumes are denoted by $\mathcal{V}_i, i = 1, 2$ and the outwards pointing unit normal of $\mathcal{V}$ is denoted by $\mathbf{n}$. Pointing from $\mathcal{V}_1$ to $\mathcal{V}_2$ the unit normal of $\mathcal{S}$ is denoted by $\boldsymbol{\nu}$. The unit normal $\mathbf{n}_\mathcal{S}$ is tangential to $\mathcal{S}$ but normal to $\partial\mathcal{S}$.

As mentioned before $\partial\mathcal{V}$ is a material surfaces in contrast to $\mathcal{S}$ which allows mass transfer between the two regions.
A general balance equation for an additive physical quantity Ψ states that the total change in time is equal to the flux across the boundary and the (internal) sources [3], i.e.

$$\frac{\mathrm{d}\Psi}{\mathrm{d}t} = \underbrace{\Phi}_{\text{Flux}} + \underbrace{\Xi}_{\text{Source}} . \tag{2.1}$$

In the case of a zero right hand side equation (2.1) becomes a conservation law. For the generic quantity Ψ we have the corresponding volume density ψ and the surface density $\psi_\mathcal{S}$. Thus Ψ may be written as

$$\Psi(t) = \int\limits_{\mathcal{V}_1 \cup \mathcal{V}_2} \psi \, \mathrm{d}V + \int\limits_{\mathcal{S}} \psi_\mathcal{S} \, \mathrm{d}A. \tag{2.2}$$

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[2] With particle one does not actually refer to the molecules or atoms of the material. Instead a particle is the smallest partition of the material such that microscopic effects can be neglected and a continuous description is possible.

[3] In the following we will highlight the equations using two colors to highlight the contributions to the resulting equations.

In a similar manner we introduce the volume flux density $\boldsymbol{\phi}$ and the surface flux density $\boldsymbol{\phi}_{\mathcal{S}}$ and write (see [21, 64])

$$\Phi(t) = -\int_{(\partial\mathcal{V}_1\cup\partial\mathcal{V}_2)\setminus\mathcal{S}} \boldsymbol{\phi}\cdot\mathbf{n}\,\mathrm{d}A - \int_{\partial\mathcal{S}} \boldsymbol{\phi}_{\mathcal{S}}\cdot\mathbf{n}_{\mathcal{S}}\,\mathrm{d}l. \tag{2.3}$$

The first integral accounts for the non-convective flux across the closed surface of the material volume. Whereas the second integral describes the flux which is tangential to $\mathcal{S}$ and normal to its closed boundary $\partial\mathcal{S}$. Since the normal vectors $\mathbf{n}$ and $\mathbf{n}_{\mathcal{S}}$ are pointing outwards, the sign takes care that incoming fluxes contribute positively to Φ.
The source Ξ can be decomposed using the volume density ξ and the surface density $\xi_{\mathcal{S}}$ and thus

$$\Xi(t) = \int_{\mathcal{V}_1\cup\mathcal{V}_2} \xi\,\mathrm{d}V + \int_{\mathcal{S}} \xi_{\mathcal{S}}\,\mathrm{d}A. \tag{2.4}$$

Inserting equations (2.2), (2.3) and (2.4) into the general balance law (2.1) gives

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_{\mathcal{V}_1\cup\mathcal{V}_2} \psi\,\mathrm{d}V + \int_{\mathcal{S}} \psi_{\mathcal{S}}\,\mathrm{d}A\right)\\ &= -\int_{(\partial\mathcal{V}_1\cup\partial\mathcal{V}_2)\setminus\mathcal{S}} \boldsymbol{\phi}\cdot\mathbf{n}\,\mathrm{d}A - \int_{\partial\mathcal{S}} \boldsymbol{\phi}_{\mathcal{S}}\cdot\mathbf{n}_{\mathcal{S}}\,\mathrm{d}l + \int_{\mathcal{V}_1\cup\mathcal{V}_2} \xi\,\mathrm{d}V + \int_{\mathcal{S}} \xi_{\mathcal{S}}\,\mathrm{d}A.\end{aligned} \tag{2.5}$$

Examples for physical quantities and their corresponding densities may be found in [21] or (with slight differences (!)) summarized in a table in [64].
The basic assumption that surface quantities contribute to the total quantity Ψ is a major point. In fact, this assumption will be responsible for additional terms in the equations for singular points, which are absent in the standard case where the jump conditions are purely algebraic.
In the following the time derivative on the left hand side of equation (2.5) is evaluated using transport theorems since the volume also depends on time. To this end we start with Reynolds' transport theorem for volume integrals.

Theorem 2.1.1 (Reynolds' Transport Theorem)**.** *Let* $\psi : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}$ *be a continuously differentiable density function and* $\mathcal{V}(t) \in \mathbb{R}^n$ *be a closed volume moving with the (particle) velocity* $\mathbf{v}$*. Then the following holds*

$$\frac{\mathrm{d}}{\mathrm{d}t}\Psi(t) = \frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{V}(t)} \psi(t,\mathbf{x})\,\mathrm{d}V = \int\limits_{\mathcal{V}(t)} \left[\frac{\partial}{\partial t}\psi(t,\mathbf{x}) + \nabla_x \cdot (\psi(t,\mathbf{x})\mathbf{v})\right] \mathrm{d}V. \tag{2.6}$$

Proof: Detailed proofs may be found in [2] and [85]. The key idea is that at any time the volume $\mathcal{V}(t)$ may be described applying a smooth transformation to the initial volume $\mathcal{V}(0)$. Let the initial volume $\mathcal{V}(0)$ be described using the coordinates $\mathbf{X} = (X_1, \dots, X_n)$. Since we consider a closed (or material) volume no particles are destroyed or added in the volume. Thus we assume the existence of a diffeomorphism $\chi(t,\mathbf{X})$ such that at every time $t \geq 0$ the coordinates $\mathbf{x}$ are given by $\mathbf{x} = \chi(t,\mathbf{X})$. For $t = 0$ the mapping χ is the identity. The Jacobian of χ for fixed t is given by $\mathbf{D}\chi(t,\mathbf{X}) = \left(\partial\chi_i/\partial X_j\right)_{i,j}$ and let $J = \det(\mathbf{D}\chi)$ denote the corresponding determinant. The determinant J is needed to relate the present volume element $\mathrm{d}V$ to the volume element of the initial configuration $\mathrm{d}V_0$, i.e. $\mathrm{d}V = J\mathrm{d}V_0$. Since J is a function of time we may calculate the time derivative and obtain (see [2, 85])

$$\frac{\mathrm{d}J}{\mathrm{d}t} = J\nabla \cdot \mathbf{v}.$$

Now we obtain

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\Psi(t) &= \frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{V}(t)} \psi(t,\mathbf{x})\,\mathrm{d}V = \frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{V}(0)} \psi(t,\chi(t,\mathbf{X}))J\,\mathrm{d}V_0 \\
&= \int\limits_{\mathcal{V}(0)} \frac{\mathrm{d}}{\mathrm{d}t}\left(\psi(t,\chi(t,\mathbf{X}))J\right)\,\mathrm{d}V_0 \\
&= \int\limits_{\mathcal{V}(0)} \left[\frac{\mathrm{d}}{\mathrm{d}t}\psi(t,\chi(t,\mathbf{X})) + \psi(t,\chi(t,\mathbf{X}))\nabla \cdot \mathbf{v}\right] J\,\mathrm{d}V_0 \\
&= \int\limits_{\mathcal{V}(t)} \left[\frac{\mathrm{d}}{\mathrm{d}t}\psi(t,\mathbf{x}) + \psi(t,\mathbf{x})\nabla \cdot \mathbf{v}\right] \mathrm{d}V.
\end{aligned}$$

Using the chain rule and $\mathbf{v} = \mathrm{d}\mathbf{x}/\mathrm{d}t = \partial\chi(t,\mathbf{X})/\partial t$ we may also write

$$\frac{\mathrm{d}}{\mathrm{d}t}\Psi(t) = \frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{V}(t)} \psi(t,\mathbf{x})\,\mathrm{d}V = \int\limits_{\mathcal{V}(t)} \left[\frac{\partial}{\partial t}\psi(t,\mathbf{x}) + \nabla_x \cdot (\psi(t,\mathbf{x})\mathbf{v})\right] \mathrm{d}V.$$

□

Since we are concerned with a situation where the volume is divided into two due to the presence of an internal surface, we want to give a generalization of Theorem 2.1.1. To keep the notation compact, we introduce the jump brackets $[\![.]\!]$. Consider the situation of Figure 2.1 and a function which is continuous in $\mathcal{V}_1 \cup \mathcal{V}_2$. For points $\mathbf{x}_\mathcal{S} \in \mathcal{S}$ we write

$$f_i(t,\mathbf{x}_\mathcal{S}) = \lim_{\mathcal{V}_i \ni \mathbf{x} \to \mathbf{x}_\mathcal{S}} f(t,\mathbf{x}),\ i = 1,2 \quad \text{and} \quad [\![f]\!]\,(t,\mathbf{x}_\mathcal{S}) := f_2(t,\mathbf{x}_\mathcal{S}) - f_1(t,\mathbf{x}_\mathcal{S}).$$

Usually we will not write out the argument since either the equations containing jump brackets should hold in any point of the surface or it is clear from the context which point is meant.

Theorem 2.1.2 (Generalized Reynolds' Transport Theorem)**.**

(i) Let Ω be an arbitrary volume (such that Gauss' theorem can be applied) and $\psi : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}$ be a continuously differentiable density function. Then the following equation holds

$$\int\limits_{\Omega} \left[\frac{\partial}{\partial t}\psi(t,\mathbf{x}) + \nabla_x \cdot (\psi(t,\mathbf{x})\mathbf{v})\right] \mathrm{d}V = \int\limits_{\Omega} \frac{\partial}{\partial t}\psi(t,\mathbf{x})\,\mathrm{d}V + \int\limits_{\partial\Omega} \psi(t,\mathbf{x})\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}A. \tag{2.7}$$

*(ii) Let Ω be a volume analogue to the situation in Figure 2.1 and Σ the internal ($n-1$-dimensional) surface. The function $\psi : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable in $\Omega_1 \cup \Omega_2$ and discontinuous across Σ. Let the velocity field be given such that it is **v** on the boundary of $\Omega_i \backslash \Sigma$ and **w** on Σ. Then the following generalization of the above equation holds*

$$\int\limits_{\Omega} \left[\frac{\partial}{\partial t}\psi(t,\mathbf{x}) + \nabla_x \cdot (\psi(t,\mathbf{x})\mathbf{v})\right] \mathrm{d}V$$

$$= \int\limits_{\Omega_1\cup\Omega_2} \frac{\partial}{\partial t}\psi(t,\mathbf{x})\,\mathrm{d}V + \int\limits_{(\partial\Omega_1\cup\partial\Omega_2)\backslash\Sigma} \psi(t,\mathbf{x})\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}A - \int\limits_{\Sigma} [\![\psi]\!]\,\mathbf{w}\cdot\boldsymbol{\nu}\,\mathrm{d}A. \tag{2.8}$$

Proof: A proof of this extension of Theorem 2.1.1 may be found in [79] (§ **C.V** pp. 525-526). The proof relies on Theorem 2.1.1 which is applied to each partial volume, now with the internal surface as part of the boundary, with a velocity field respecting the different boundary velocities **v** and **w**. Summation gives the desired result. □

Theorem 2.1.2 allows another interpretation of equation (2.6). The proof of 2.1.1 revealed that the total change of a quantity is balanced by the local change of the density function and two additional effects. First there is the convective part and second there is a contribution due to the deformation of the material volume.
An alternative interpretation can be obtained if we consider Ω to be the spatial configuration[4] of $\mathcal{V}(t)$ at a fixed time. Now Ω can be thought of as a fixed reference volume which is not material anymore and thus allows transport across its boundary. Hence we may say that the total change at time t is balanced by the local change and the flux across the boundary of Ω.

Next we need two integral identities for the (moving) surface $\mathcal{S}$, i.e. a transport theorem and a divergence theorem. We want to focus on the results rather than the mathematical description of moving surfaces in $\mathbb{R}^3$, which we will keep short. For details we recommend, as before, the books [2, 64] and further the book of Grinfeld [34]. Additional results may be found in Cermelli et al. [13]. In particular for the transport equation we also refer to [26] and the detailed description therein. A compact presentation of some helpful results is given in the Appendix 8.1.

Theorem 2.1.3 (Integral Theorems for Surfaces)**.**

(i) Let $\mathcal{S}(t), t \in [0, T_0]$ *be a family of smooth surfaces in* $\mathbb{R}^3$ *with the surface area element* $\mathrm{d}A = \sqrt{g}\mathrm{d}u^1\mathrm{d}u^2$*. Here* $g = g(t)$ *denotes the determinant of the metric tensor of the surface at time t and the surface coordinates are* $(u^1, u^2) \in \mathcal{U}$*. Further let* $\psi_{\mathcal{S}} = \psi_{\mathcal{S}}(t, \mathbf{x})$ *be a function defined on the surface such that all of the following quantities exist. The material time derivative of a surface quantity is given by* $\mathring{\psi}_{\mathcal{S}} = \partial_t \psi_{\mathcal{S}} + \mathbf{w} \cdot \nabla_x \psi_{\mathcal{S}}$*, with* $\mathbf{w}$ *beeing the velocity field of the surface particles. The transport theorem for the surface*

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[4] This notion is due to [79].

integral then reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{S}(t)} \psi_{\mathcal{S}}\,\mathrm{d}A = \int\limits_{\mathcal{S}(t)} \mathring{\psi}_{\mathcal{S}} + \psi_{\mathcal{S}}\frac{1}{2g}\frac{\partial}{\partial t}g\,\mathrm{d}A. \tag{2.9}$$

The time derivative of g is given by (8.24).

(ii) Let $\mathcal{S} \subset \mathbb{R}^3$ be a smooth surface with the outward pointing boundary normal $\mathbf{n}_{\mathcal{S}}$ tangential to the surface. Further $\boldsymbol{\phi}_{\mathcal{S}}$ is a continuously differentiable vector field. This function may be decomposed as follows $\boldsymbol{\phi}_{\mathcal{S}} = \phi_\tau^\alpha \boldsymbol{\tau}_\alpha + \phi_\nu \boldsymbol{\nu}$ into tangential and normal components. Then the divergence theorem for surface integrals holds

$$\int\limits_{\partial\mathcal{S}} \boldsymbol{\phi}_{\mathcal{S}} \cdot \mathbf{n}_{\mathcal{S}}\,\mathrm{d}l = \int\limits_{\mathcal{S}} \nabla_\alpha \boldsymbol{\phi}_\tau^\alpha\,\mathrm{d}A. \tag{2.10}$$

Proof: Part (i): The proof of the transport theorem for the surface is quite analogue to the proof of Theorem 2.1.1. According to the results presented in 8.1 we have to account for two mappings. First we go from the current surface $\mathcal{S}(t)$ to the initial configuration $\mathcal{S}(0)$ and then down to the surface coordinates. This mapping is given by $\tilde{\Phi} : \mathcal{U} \to \mathcal{S}(t)$, see 8.1. We obtain

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{S}(t)} \psi_{\mathcal{S}}(t,\mathbf{x})\,\mathrm{d}A &= \frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{\mathcal{U}} \psi_{\mathcal{S}}(t,\tilde{\Phi}(t,u^\alpha))\,\sqrt{g}\,\mathrm{d}u^1\mathrm{d}u^2 \\
&= \int\limits_{\mathcal{U}} \left(\frac{\mathrm{d}}{\mathrm{d}t}\psi_{\mathcal{S}}(t,\tilde{\Phi}(t,u^\alpha)) + \psi_{\mathcal{S}}\frac{1}{2g}\frac{\partial}{\partial t}g\right)\sqrt{g}\,\mathrm{d}u^1\mathrm{d}u^2 \\
&= \int\limits_{\mathcal{S}(t)} \mathring{\psi}_{\mathcal{S}} + \psi_{\mathcal{S}}\frac{1}{2g}\frac{\partial}{\partial t}g\,\mathrm{d}A.
\end{aligned} \tag{2.11}$$

For the last line we used that $\psi_{\mathcal{S}}$ is a function of $(t,\mathbf{x})$ with $\mathbf{x} = \tilde{\Phi}(t,u^1,u^2)$ as in 8.1 with $\mathbf{w} = \mathrm{d}\mathbf{x}/\mathrm{d}t$.

Part (ii): We will just sketch the proof of the second statement here, but a detailed one may be found in [2] and [64]. The first major point is the observation that Stokes' theorem for the surface may be written as

$$\int_{\mathcal{S}} \varepsilon^{\alpha\beta}\nabla_\alpha A_\beta\,\mathrm{d}A = \int_{\partial\mathcal{S}} A_\beta \bar{\boldsymbol{\tau}}^\beta\,\mathrm{d}l$$

Here $\bar{\boldsymbol{\tau}}^\beta$ denotes the *unit surface vector tangent to the curve $\partial\mathcal{S}$*. Further we have

$$\varepsilon_{\alpha\beta} = \sqrt{g}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \text{with} \quad \varepsilon_{\alpha\gamma}\varepsilon^{\gamma\beta} = \delta^\alpha_\beta.$$

Now with the choice $A_\beta = \varepsilon_{\beta\gamma}B^\gamma$ one yields $\varepsilon^{\alpha\beta}\nabla_\alpha A_\beta = \nabla_\alpha B^\alpha$. Further $\varepsilon_{\beta\gamma}\bar{\boldsymbol{\tau}}^\beta = \bar{\boldsymbol{\nu}}_\gamma$ is the *outward unit normal to the curve $\partial\mathcal{S}$ in the surface*. For this special choice Stokes' theorem reads

$$\int_{\mathcal{S}} \nabla_\alpha B^\alpha \,\mathrm{d}A = \int_{\partial\mathcal{S}} B^\alpha \bar{\boldsymbol{\nu}}_\alpha \,\mathrm{d}l. \tag{2.12}$$

If we now consider the surface flux and decompose it in its tangential and normal components we have $\boldsymbol{\phi}_{\mathcal{S}} = \phi^\alpha_\tau \boldsymbol{\tau}_\alpha + \phi_\nu \boldsymbol{\nu}$. Further the vector $\mathbf{n}_{\mathcal{S}}$ is tangential to the surface and normal to its boundary thus may be written as $\mathbf{n}_{\mathcal{S}} = \bar{\boldsymbol{\nu}}^\alpha \boldsymbol{\tau}_\alpha$. Hence we yield $\boldsymbol{\phi}_{\mathcal{S}} \cdot \mathbf{n}_{\mathcal{S}} = \phi^\alpha_\tau \bar{\boldsymbol{\nu}}^\beta g_{\alpha\beta} = \phi^\alpha_\tau \bar{\boldsymbol{\nu}}_\alpha$. Now applying (2.12) with $B^\alpha = \phi^\alpha_\tau$ gives the desired result. ☐

Remark 2.1.4. *We want to give some few comments on the previous proof.*

(i) The proof of formula (2.9) can be found in [2] and [26]. Here, in contrast to [21, 64], the surface function depends on the surface points $\mathbf{x} \in \mathcal{S} \subset \mathbb{R}^3$.

(ii) The proof of the transport theorem in the version presented in [21, 64] can be found in [64] (§ 3.1.1.3, p. 50). There the function $\psi_{\mathcal{S}}$ directly depends on the u^α instead of the spatial surface coordinates $\mathbf{x} \in \mathcal{S} \subset \mathbb{R}^3$, i.e. $\psi_{\mathcal{S}} = \psi_{\mathcal{S}}(t, u^\alpha)$. Thus the proofs simplifies accordingly. Note, that for this reason the surface quantities in the local balance laws depend on the surface coordinates u^α instead of the corresponding space coordinates.

(iii) The proof in [2] takes into account that the surface coordinates may also be convected and thus a more general formula is obtained. This results in an additional divergence term. Here we consider surfaces with a material boundary and thus have fixed surface coordinates.

(iv) Since we assume $\psi_{\mathcal{S}}$ to be a function taking values on the surface we do not consider values away from the surface [5]. Thus we have $\mathbf{w} \cdot \nabla_x \psi_{\mathcal{S}} = w^\alpha_\tau \nabla_\alpha \psi_{\mathcal{S}}$ with the tangential components w^α_τ, see [2, 26].

---

[5] Another possibility is to consider a constant extension of $\psi_{\mathcal{S}}$ in normal direction which also would lead to a vanishing normal derivative.

(v) *In [26] a level set description of the surface is used. The resulting transport theorem is the same. In particular note that the time derivative of the metric corresponds to the surface divergence of the velocity field* **w**. *This highlights that the surface transport theorem is analogue to Reynolds' transport theorem (material time derivative of a quantity plus the quantity times the divergence of the velocity field).*

Both Theorems 2.1.1 and 2.1.3 can be used to reformulate equation (2.5). Altogether we have

$$\int\limits_{\mathcal{V}_1\cup\mathcal{V}_2} \frac{\partial}{\partial t}\psi + \nabla_x\cdot(\psi\mathbf{v})\,\mathrm{d}V + \int\limits_{\mathcal{S}} \mathring{\psi}_{\mathcal{S}} + \psi_{\mathcal{S}}\frac{1}{2g}\frac{\partial}{\partial t}g\,\mathrm{d}A$$
$$= -\int\limits_{(\partial\mathcal{V}_1\cup\partial\mathcal{V}_2)\setminus\mathcal{S}} \boldsymbol{\phi}\cdot\mathbf{n}\,\mathrm{d}A - \int\limits_{\partial\mathcal{S}} \boldsymbol{\phi}_{\mathcal{S}}\cdot\mathbf{n}_{\mathcal{S}}\,\mathrm{d}l + \int\limits_{\mathcal{V}_1\cup\mathcal{V}_2} \xi\,\mathrm{d}V + \int\limits_{\mathcal{S}} \xi_{\mathcal{S}}\,\mathrm{d}A.$$

The balance law should hold at any time for every material volume. Thus the balance law in regular points, i.e. points in $\mathcal{V}_1\cup\mathcal{V}_2$, can be obtained using an arbitrary control volume Ω contained in either one of the volumes. Therefore one may use Gauss' theorem for the boundary terms. Further the integrals with respect to the singular surface vanish. This gives

$$\int\limits_{\Omega} \frac{\partial}{\partial t}\psi + \nabla_x\cdot(\psi\mathbf{v})\,\mathrm{d}V = -\int\limits_{\partial\Omega} \boldsymbol{\phi}\cdot\mathbf{n}\,\mathrm{d}A + \int\limits_{\Omega} \xi\,\mathrm{d}V$$
$$\Leftrightarrow$$
$$\int\limits_{\Omega} \frac{\partial}{\partial t}\psi + \nabla_x\cdot(\psi\mathbf{v}+\boldsymbol{\phi})\,\mathrm{d}V = \int\limits_{\Omega} \xi\,\mathrm{d}V.$$

Since this equation should hold for arbitrary control volumes we conclude

$$\frac{\partial}{\partial t}\psi + \nabla_x\cdot(\psi\mathbf{v}+\boldsymbol{\phi}) = \xi. \tag{2.13}$$

To obtain the balance equation for the singular points, one uses a so called *pillbox argument*, for details see [64] and for the two dimensional case see [36]. The idea is to choose a cylinder Ω_ε which is oriented according to the surface normal $\boldsymbol{\nu}$ as control volume. It may be chosen as sketched in Figure 2.2. Now as ε goes to zero the volume terms vanish and the boundary terms

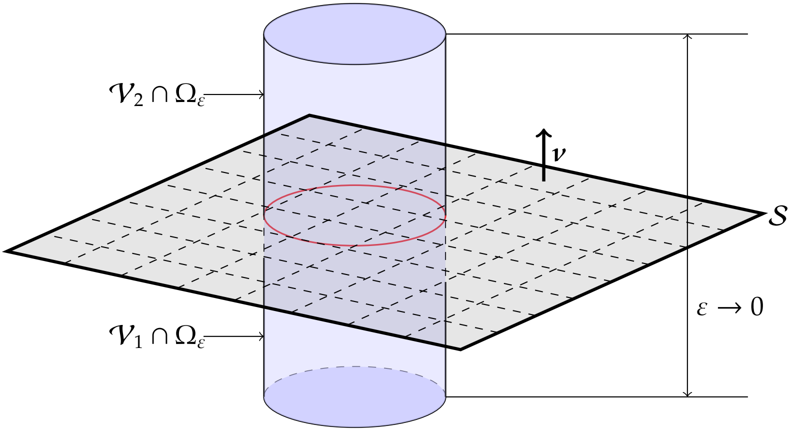

Figure 2.2: Sketch of the pillbox argument.

reduce to $\mathcal{S}_\varepsilon = \Omega_\varepsilon \cap \mathcal{S}$ with the normal $\pm\boldsymbol{\nu}$ and we obtain

$$\begin{aligned} &\int\limits_{\Omega_\varepsilon \setminus \mathcal{S}} \frac{\partial}{\partial t}\psi \,\mathrm{d}V + \int\limits_{\mathcal{S}_\varepsilon} \mathring{\psi}_{\mathcal{S}} + \psi_{\mathcal{S}} \frac{1}{2g}\frac{\partial}{\partial t} g \,\mathrm{d}A + \int\limits_{\mathcal{S}_\varepsilon} \nabla_\alpha \boldsymbol{\phi}^\alpha_\tau \,\mathrm{d}A \\ &= - \int\limits_{\partial(\mathcal{V}_1 \cap \Omega_\varepsilon)} \psi \mathbf{v} \cdot \mathbf{n}_\varepsilon \,\mathrm{d}A - \int\limits_{\partial(\mathcal{V}_2 \cap \Omega_\varepsilon)} \psi \mathbf{v} \cdot \mathbf{n}_\varepsilon \,\mathrm{d}A - \int\limits_{\partial(\mathcal{V}_1 \cap \Omega_\varepsilon)} \boldsymbol{\phi} \cdot \mathbf{n}_\varepsilon \,\mathrm{d}A \\ &\quad - \int\limits_{\partial(\mathcal{V}_2 \cap \Omega_\varepsilon)} \boldsymbol{\phi} \cdot \mathbf{n}_\varepsilon \,\mathrm{d}A + \int\limits_{\mathcal{S}_\varepsilon} [\![\psi]\!] \,\mathbf{w} \cdot \boldsymbol{\nu} \,\mathrm{d}A + \int\limits_{\Omega_\varepsilon \setminus \mathcal{S}} \xi \,\mathrm{d}V + \int\limits_{\mathcal{S}_\varepsilon} \xi_{\mathcal{S}} \,\mathrm{d}A \\ &\overset{\varepsilon \to 0}{\Rightarrow} \\ &\int\limits_{\mathcal{S}_\varepsilon} \left(\mathring{\psi}_{\mathcal{S}} + \psi_{\mathcal{S}} \frac{1}{2g}\frac{\partial}{\partial t} g + \nabla_\alpha \boldsymbol{\phi}^\alpha_\tau \right) \mathrm{d}A = \int\limits_{\mathcal{S}_\varepsilon} \left([\![\psi]\!] \,\mathbf{w} \cdot \boldsymbol{\nu} - [\![\psi \mathbf{v} + \boldsymbol{\phi}]\!] \cdot \boldsymbol{\nu} + \xi_{\mathcal{S}} \right) \mathrm{d}A \end{aligned}$$

Thus one obtains together with (8.24) the local balance law in points on the surface

$$\mathring{\psi}_{\mathcal{S}} + \psi_{\mathcal{S}} \left(\nabla_\alpha w^\alpha_\tau - 2K_M w_\nu \right) + \nabla_\alpha \phi^\alpha_\tau = w_\nu \,[\![\psi]\!] - [\![\psi \mathbf{v} + \boldsymbol{\phi}]\!] \,\boldsymbol{\nu} + \xi_{\mathcal{S}}. \tag{2.14}$$

The left hand side of (2.14) is the "non-classical part" of the jump conditions and is due to the assignment of a surface quantity.

So far we derived the equations in three dimensions but the lower dimensional cases may also be derived from these equations. In particular we focus on (2.14). We briefly want to *sketch* how this may be done, but of course one may derive these cases on their own.
Assume we have a symmetry such that the surface density is constant in one surface direction and the normal has no component in this direction. For example we may choose our coordinate system such that the density is constant in (w.l.o.g.) x_3 direction and the surface normal has the x_3 component zero. Then the problem reduces to a two dimensional problem, where the singular surface reduces to a curve. The remaining surface coordinate may be interpreted as the *arc-length s* of the curve. Further the mean curvature, as sum of the principle curvatures, reduces to $K_M = \kappa/2$. Finally the divergence of the tangential component of the surface velocity reduces to the derivative with respect to the *arc-length s*. Thus we obtain

$$\mathring{\psi}_{\mathcal{S}}(t,s) + \psi_{\mathcal{S}}\left(\frac{\partial}{\partial s}w_\tau - \kappa w_\nu\right) + \frac{\partial}{\partial s}\phi_\tau = w_\nu \left[\!\left[\psi\right]\!\right] - \left[\!\left[\psi\mathbf{v} + \boldsymbol{\phi}\right]\!\right] \boldsymbol{\nu} + \xi_{\mathcal{S}}. \tag{2.15}$$

A detailed derivation, which is genuine two dimensional, is given in the book of Gurtin [36].
Now for the one dimensional case we assume a planar interface (which stays planar) with a spatially constant surface density. Since the metric is constant in time, the derivative $\partial_t g$ vanishes and thus we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\psi_{\mathcal{S}}(t) = w_\nu \left[\!\left[\psi\right]\!\right] - \left[\!\left[\psi v + \phi\right]\!\right] + \xi_{\mathcal{S}}. \tag{2.16}$$

This type of jump condition is also known as *generalized Rankine-Hugoniot jump conditions*, cf. Yang [86].

2.2 Specific Balance Laws & the Entropy Inequality

Throughout this work we are only interested in balance laws where the production densities ξ and $\xi_{\mathcal{S}}$ are identically zero. Often these equations are referred to as conservation laws, although strictly speaking the considered quantities might not be conserved due to the presence of a non-convective flux. For example see the balance of momentum 2.2.2. In particular there are four quantities we are interested in. These are *mass, momentum* and *(total) energy*. Further we want to derive the inequality for the *entropy*. Together these four reflect the following four physical principles

(I) Conservation of Mass

(II) Newton's second law

(III) First law of thermodynamics (1.1.2)

(IV) Second law of thermodynamics (1.1.3)

Since we are only interested in fluids with certain properties (e.g. non-viscous) we will assume some (physical) simplifications. We will make the reader aware of such situations. As already mentioned before, results for other quantities may be obtained using [21] and [64]. A very recent work by Bothe & Dreyer [11] contains a very broad description of continuum thermodynamics for multicomponent fluids with focus on chemical reactions. In [11] various theoretical approaches and their difference are discussed. Further they deal with constitutive modeling and the entropy principle and compare the presented approach to the one (among others) discussed in [64].

2.2.1 Conservation of Mass

In order to obtain the conservation law of mass we make the following choices

Ψ	ψ	$\boldsymbol{\phi}$	ξ	$\psi_{\mathcal{S}}$	ϕ_τ^α	$\xi_{\mathcal{S}}$
mass	ρ	0	0	$\rho_{\mathcal{S}}$	0	0

$$\frac{\partial}{\partial t}\rho + \nabla_x \cdot (\rho \mathbf{v}) = 0, \tag{2.17}$$

$$\mathring{\rho}_{\mathcal{S}}(t, \mathbf{x}) + \rho_{\mathcal{S}}\left(\nabla_\alpha w_\tau^\alpha - 2K_M w_\nu\right) - [\![\rho(\mathbf{w} - \mathbf{v})]\!] \cdot \boldsymbol{\nu} = 0. \tag{2.18}$$

For the following we introduce the mass flux $\dot{m} = \rho(\mathbf{v} - \mathbf{w}) \cdot \boldsymbol{\nu}$ and thus can rewrite (2.18)

$$\mathring{\rho}_{\mathcal{S}}(t, \mathbf{x}) + \rho_{\mathcal{S}}\left(\nabla_\alpha w_\tau^\alpha - 2K_M w_\nu\right) = -[\![\dot{m}]\!]\,. \tag{2.19}$$

Note that (2.17) follows immediately from the classical version of Reynolds Transport Theorem 2.1.1. A nice interpretation of the curvature term in (2.19) is given in [64].

2.2.2 Balance of Momentum

Before we present the balance laws of momentum we want to simplify the physics. For the momentum (precisely the i^{th} component $i \in \{1, 2, 3\}$) we have a non-convective flux which is in general given by $\boldsymbol{\phi} = -\mathbf{t}_{ik}$. Here $\mathbf{t}_{ik}$ is the *Cauchy Stress Tensor* with $i, k \in \{1, 2, 3\}$. In the following we only consider (isotropic) *non-viscous fluids* and thus the stress tensor simplifies to $\mathbf{t}_{ik} = -p\delta_{ik}$, with p being the pressure. The surface flux is related to the surface stress which is given by the *Second Piola Kirchhoff Stress* $\mathbf{t}_{\mathcal{S}}^{i\alpha}$. This stress acts on the surface and is a *force per line*. It may be decomposed in a tangential and a normal part, i.e.

$$\mathbf{t}_{\mathcal{S}}^{i\alpha} = S^{\alpha\beta}\boldsymbol{\tau}_{\beta}^{i} + S^{\alpha}\boldsymbol{\nu}^{i}. \tag{2.20}$$

Now we assume that the surface balances external forces only by tangential stresses, which is reasonable for a liquid-vapor phase interface. Thus the surface deforms when exposed to external loads. Models with this assumptions are also called *membrane* model, see [21, 64]. The important consequence is, that the surface stress is symmetric whereas the normal stress vanishes, i.e.

$$S^{\alpha\beta} = S^{\beta\alpha} \quad \text{and} \quad S^{\alpha} = 0.$$

In particular we have $\phi_{\tau}^{\alpha} = -\mathbf{t}_{\mathcal{S}}^{i\alpha}$. Now we have everything at hand to write down the balance laws for the following choice of variables (for $i \in \{1, 2, 3\}$)

Ψ	ψ	ϕ	ξ	$\psi_{\mathcal{S}}$	ϕ_{τ}^{α}	$\xi_{\mathcal{S}}$
momentum	$\rho\mathbf{v}_i$	$p\mathbf{e}^{(\mathbf{i})}$[6]	0	$\rho_{\mathcal{S}}\mathbf{w}_i$	$-\mathbf{t}_{\mathcal{S}}^{i\alpha}$	0

$$\frac{\partial}{\partial t}(\rho\mathbf{v}_i) + \nabla_x \cdot \left(\rho\mathbf{v}_i\mathbf{v} + p\mathbf{e}^{(\mathbf{i})}\right) = 0, \tag{2.21}$$

$$(\rho_{\mathcal{S}}\overset{\circ}{\mathbf{w}}_i) + \rho_{\mathcal{S}}\mathbf{w}_i\left(\nabla_{\alpha}w_{\tau}^{\alpha} - 2K_M w_{\nu}\right) - \nabla_{\alpha}\mathbf{t}_{\mathcal{S}}^{i\alpha} = w_{\nu}\,[\![\rho\mathbf{v}_i]\!] - \left[\!\left[\rho\mathbf{v}_i\mathbf{v} + p\mathbf{e}^{(\mathbf{i})}\right]\!\right] \cdot \boldsymbol{\nu}. \tag{2.22}$$

---

[6] $\mathbf{e}^{(\mathbf{1})} = (1, 0, 0)$, $\mathbf{e}^{(\mathbf{2})} = (0, 1, 0)$, $\mathbf{e}^{(\mathbf{3})} = (0, 0, 1)$

Using (2.19) the second equation can be simplified as follows

$$
\begin{aligned}
&(\rho_{\mathcal{S}}\mathring{\mathbf{w}}_i) + \rho_{\mathcal{S}}\mathbf{w}_i \left(\nabla_\alpha w_\tau^\alpha - 2K_M w_\nu\right) - \nabla_\alpha \mathbf{t}_{\mathcal{S}}^{i\alpha} = w_\nu \llbracket \rho\mathbf{v}_i \rrbracket - \left\llbracket \rho\mathbf{v}_i\mathbf{v} + p\mathbf{e}^{(\mathbf{i})} \right\rrbracket \cdot \boldsymbol{\nu} \\
&\overset{(2.19)}{\Leftrightarrow} \\
&(\rho_{\mathcal{S}}\mathring{\mathbf{w}}_i) - \mathbf{w}_i \left(\mathring{\rho}_{\mathcal{S}} + \llbracket \dot{m} \rrbracket\right) - \nabla_\alpha \mathbf{t}_{\mathcal{S}}^{i\alpha} = \llbracket \rho\mathbf{v}_i(\mathbf{w} - \mathbf{v}) \rrbracket \cdot \boldsymbol{\nu} - \llbracket p \rrbracket \boldsymbol{\nu}_i \\
&\Leftrightarrow \\
&\rho_{\mathcal{S}}\mathring{\mathbf{w}}_i - \mathbf{w}_i \llbracket \dot{m} \rrbracket - \nabla_\alpha \mathbf{t}_{\mathcal{S}}^{i\alpha} = -\llbracket \mathbf{v}_i\dot{m} \rrbracket - \llbracket p \rrbracket \boldsymbol{\nu}_i \\
&\Leftrightarrow \\
&\rho_{\mathcal{S}}\mathring{\mathbf{w}}_i - \nabla_\alpha \mathbf{t}_{\mathcal{S}}^{i\alpha} = -\llbracket \dot{m}(\mathbf{v}_i - \mathbf{w}_i) \rrbracket - \llbracket p \rrbracket \boldsymbol{\nu}_i,\ i \in \{1, 2, 3\}.
\end{aligned}
\tag{2.23}
$$

We further want to illustrate why equation (2.21) is referred to as Euler equation and thus is the origin of the name for the system of Euler equations. In the following we show that the original Euler equation (stated by Euler in 1755, [52] §2) is implied by (2.21), provided the conservation of mass (2.17) holds. We have

$$
\begin{aligned}
0 &= \frac{\partial}{\partial t}(\rho\mathbf{v}_i) + \nabla_x \cdot \left(\rho\mathbf{v}_i\mathbf{v} + p\mathbf{e}^{(\mathbf{i})}\right) \\
&= \rho\frac{\partial}{\partial t}\mathbf{v}_i + \mathbf{v}_i\frac{\partial}{\partial t}\rho + \mathbf{v}_i\nabla_x \cdot (\rho\mathbf{v}) + \rho\mathbf{v} \cdot \nabla_x\mathbf{v}_i + \nabla_x \cdot \left(p\mathbf{e}^{(\mathbf{i})}\right) \Bigg| \cdot \mathbf{v}_i \Bigg| \sum_{i=1}^{3} \\
0 &= \mathbf{v}^2 \underbrace{\left(\frac{\partial}{\partial t}\rho + \nabla_x \cdot (\rho\mathbf{v})\right)}_{\overset{(2.17)}{=} 0} + \rho\mathbf{v} \cdot \left(\frac{\partial}{\partial t}\mathbf{v} + \frac{1}{2}\nabla_x\mathbf{v}^2 + \frac{1}{\rho}\nabla_x p\right) \\
&\Leftrightarrow \\
&\frac{\partial}{\partial t}\mathbf{v} + \frac{1}{2}\nabla_x\mathbf{v}^2 = -\frac{1}{\rho}\nabla_x p.
\end{aligned}
\tag{2.24}
$$

In [52] this equation is obtained from

$$
\rho\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\nabla_x p.
$$

This is Newton's second law applied to a volume element of the fluid, as it was considered by Euler. On the left hand side we have the density ρ times the acceleration $\mathrm{d}\mathbf{v}/\mathrm{d}t$ which is equal to the force $-\nabla_x p$ acting on the volume

element.
A further result is obtained if we first multiply (2.21) by $\mathbf{v}_i$ and then calculate the sum for $i = 1, 2, 3$. This gives the balance law for the *kinetic energy*

$$\frac{\partial}{\partial t}\left(\rho\frac{\mathbf{v}^2}{2}\right) + \nabla_x \cdot \left(\frac{1}{2}\rho\mathbf{v}^2\mathbf{v} + p\mathbf{v}\right) = p\nabla_x \cdot \mathbf{v}. \tag{2.25}$$

The analogue equation for the singular points can be obtained accordingly, i.e.

$$\begin{aligned} \rho_{\mathcal{S}}\mathring{\mathbf{w}}_i - \nabla_\alpha \mathbf{t}^{i\alpha}_{\mathcal{S}} &= -\llbracket \dot{m}(\mathbf{v}_i - \mathbf{w}_i)\rrbracket - \llbracket p\rrbracket\, \boldsymbol{\nu}_i \,\Big|\cdot \mathbf{w}_i \,\Big|\sum_{i=1}^{3} \\ \frac{\rho_{\mathcal{S}}}{2}\mathring{\mathbf{w}}^2 - \sum_{i=1}^{3}\mathbf{w}_i\nabla_\alpha \mathbf{t}^{i\alpha}_{\mathcal{S}} &= -\llbracket \dot{m}(\mathbf{v} - \mathbf{w})\cdot\mathbf{w}\rrbracket - \llbracket p\rrbracket\, \mathbf{w}\cdot\boldsymbol{\nu} \end{aligned} \tag{2.26}$$

For further remarks see [64].

2.2.3 Balance of Energy

Now we want to derive the balance law for the total energy. Up to now the results in [21] and [64] are the same as far as our case is concerned. However, for the energy balance a major difference occurs, which for example is of importance for the isothermal Euler equations 2.4.2. The energy density in the bulk phases is given by

$$\mathcal{E} := \rho\left(e + \frac{\mathbf{v}^2}{2}\right). \tag{2.27}$$

Where e is the specific internal energy as introduced in Chapter 1. Now in slight contrast the surface energy density is given as in [21]

$$\mathcal{E}_{\mathcal{S}} := e_{\mathcal{S}} + \rho_{\mathcal{S}}\frac{\mathbf{w}^2}{2}. \tag{2.28}$$

The major difference between both is that the internal surface energy is not multiplied by the surface density. In fact this is the difference between the [21] and [64]. For the flux terms we neglect gravitational, electromagnetic contributions as well as radiation. With $\mathbf{q}$ we denote the *heat flux* in the bulk and with $\mathbf{q}^\alpha_\tau$ the *tangential surface heat flux*. Altogether we obtain

Ψ	ψ	$\boldsymbol{\phi}$	ξ	$\psi_{\mathcal{S}}$	ϕ^{α}_{τ}	$\xi_{\mathcal{S}}$
total energy	$\mathcal{E}$	$\mathbf{q}+p\mathbf{v}$	0	$\mathcal{E}_{\mathcal{S}}$	$\mathbf{q}^{\alpha}_{\tau}-\mathbf{t}^{i\alpha}_{\mathcal{S}}\mathbf{w}_i$	0

$$\frac{\partial}{\partial t}\mathcal{E}+\nabla_x\cdot\left(\mathbf{v}\left(\mathcal{E}+p\right)+\mathbf{q}\right)=0, \tag{2.29}$$

$$\mathring{\mathcal{E}}_{\mathcal{S}}+\mathcal{E}_{\mathcal{S}}\left(\nabla_\alpha w^\alpha_\tau-2K_M w_\nu\right)+\nabla_\alpha\left(\mathbf{q}^\alpha_\tau-\mathbf{t}^{i\alpha}_{\mathcal{S}}\mathbf{w}_i\right)=w_\nu[\![\mathcal{E}]\!]-[\![\mathbf{v}\left(\mathcal{E}+p\right)+\mathbf{q}]\!]\cdot\boldsymbol{\nu}. \tag{2.30}$$

Using (2.19) the second equation can be simplified as follows

$$\begin{aligned}
&\mathring{\mathcal{E}}_{\mathcal{S}}+\mathcal{E}_{\mathcal{S}}\left(\nabla_\alpha w^\alpha_\tau-2K_M w_\nu\right)+\nabla_\alpha\left(\mathbf{q}^\alpha_\tau-\mathbf{t}^{i\alpha}_{\mathcal{S}}\mathbf{w}_i\right) \qquad (2.31)\\
=\;& w_\nu\left[\!\!\left[\rho\left(e+\frac{\mathbf{v}^2}{2}\right)\right]\!\!\right]-\left[\!\!\left[\rho\mathbf{v}\left(e+\frac{\mathbf{v}^2}{2}\right)+\mathbf{q}+p\mathbf{v}\right]\!\!\right]\cdot\boldsymbol{\nu}\\
&\overset{(2.19)}{\Leftrightarrow}\\
&\mathring{\mathcal{E}}_{\mathcal{S}}+e_{\mathcal{S}}\left(\nabla_\alpha w^\alpha_\tau-2K_M w_\nu\right)-\frac{\mathbf{w}^2}{2}\left(\frac{\partial}{\partial t}\rho_{\mathcal{S}}+[\![\dot{m}]\!]\right)+\nabla_\alpha\left(\mathbf{q}^\alpha_\tau-\mathbf{t}^{i\alpha}_{\mathcal{S}}\mathbf{w}_i\right)\\
=\;&\left[\!\!\left[\rho(\mathbf{w}-\mathbf{v})\left(e+\frac{\mathbf{v}^2}{2}\right)\right]\!\!\right]\cdot\boldsymbol{\nu}-[\![\mathbf{q}+p\mathbf{v}]\!]\cdot\boldsymbol{\nu}\\
&\Leftrightarrow\\
&\mathring{e}_{\mathcal{S}}+\frac{\rho_{\mathcal{S}}}{2}(\mathring{\mathbf{w}}^2)+e_{\mathcal{S}}\left(\nabla_\alpha w^\alpha_\tau-2K_M w_\nu\right)+\nabla_\alpha\left(\mathbf{q}^\alpha_\tau-\mathbf{t}^{i\alpha}_{\mathcal{S}}\mathbf{w}_i\right)\\
=\;&-\left[\!\!\left[\dot{m}\left(e+\frac{\mathbf{v}^2-\mathbf{w}^2}{2}\right)\right]\!\!\right]-[\![\mathbf{q}+p\mathbf{v}]\!]\cdot\boldsymbol{\nu} \qquad (2.32)
\end{aligned}$$

Equation (2.32) again highlights the major impact of the particular structure of $\mathcal{E}_{\mathcal{S}}$. Since now a contribution of the surface energy $e_{\mathcal{S}}$ remains even when $\rho_{\mathcal{S}}\equiv 0$.

An alternative derivation of (2.29) and (2.30) can be given by adding the balance law of the kinetic energy and the balance law of the internal energy, see [64]. There the balance law for the *kinetic energy* is derived from the conservation laws of momentum (2.21) and (2.22). Further the balance law for the internal energy is derived, which basically represents the first law of thermodynamics 1.1.2. By adding both balance laws the conservation law for the total energy is obtained.

We want to close the discussion of the total energy by deriving the balance for the internal energy which we will use later. We obtain

$$\begin{aligned}
0 &= \frac{\partial}{\partial t}\mathcal{E} + \nabla_x \cdot (\mathbf{v}(\mathcal{E} + p) + \mathbf{q}) \\
&= \frac{\partial}{\partial t}\left[\rho\left(e + \frac{\mathbf{v}^2}{2}\right)\right] + \nabla_x \cdot \left[\mathbf{v}\left(\rho\left(e + \frac{\mathbf{v}^2}{2}\right) + p\right) + \mathbf{q}\right] \\
&= \frac{\partial}{\partial t}(\rho e) + \nabla_x \cdot (\rho e\mathbf{v} + \mathbf{q}) + \underbrace{\frac{\partial}{\partial t}\left(\rho\frac{\mathbf{v}^2}{2}\right) + \nabla_x \cdot \left(\frac{1}{2}\rho\mathbf{v}^2\mathbf{v} + p\mathbf{v}\right)}_{\overset{(2.25)}{=} p\nabla_x \cdot \mathbf{v}}
\end{aligned}$$

$$\Leftrightarrow$$

$$\frac{\partial}{\partial t}(\rho e) + \nabla_x \cdot (\rho e\mathbf{v} + \mathbf{q}) = -p\nabla_x \cdot \mathbf{v}. \tag{2.33}$$

2.2.4 Entropy Inequality

Finally we want to present the balance law for the entropy. In view of the second law of thermodynamics (1.1.3) we of course cannot expect the entropy to be conserved in general. Instead we will obtain a balance law which will reflect the Clausius inequality (1.1). A detailed discussion of the entropy principle and derivation of the balance law in other situations may be found in [11, 21] and [64]. Especially for the entropy principle applied to the bulk phases we refer to [11] and [64]. Nevertheless we want to make the reader aware of the following aspects

(i) Bothe & Dreyer [11] focus on chemical reactions in mixtures (with a common temperature) and are not concerned with interfaces.

(ii) Although we again follow [21] there are two main differences in the following. In contrast to [21] we focus on a single substance and ignore chemical reactions. Thus the non-convective entropy flux simplifies to

$$\phi = \frac{1}{T}\left(\mathbf{q} - \sum_{a=1}^{a_c} \mu_a \mathbf{J}_a\right) = \frac{\mathbf{q}}{T}. \tag{2.34}$$

Where $\mu_a \mathbf{J}_a$ denote the chemical potential and the diffusion flux of constituent a. The second notable difference is that in [21] the main focus is on situations where there is no temperature jump at the interface, i.e. $[\![T]\!] = 0$. We will not assume this in general.

(iii) We have according to [21] that the surface entropy density is given by $\psi_{\mathcal{S}} = s_{\mathcal{S}}$. As for the surface energy density (2.28) this is in contrast to [64] where density is given by $\psi_{\mathcal{S}} = \rho_{\mathcal{S}} s_{\mathcal{S}}$.

(iv) In [64] the entropy principle for singular surfaces is applied to an *ideal wall* and thus there is no mass flux across the interface.

As mentioned before we have production terms for the entropy in the bulk and on the surface. For our purposes it is sufficient to know that the production terms are positive. Detailed discussions of the production terms my be found in [11, 51, 59, 64] and [70]. We obtain

Ψ	ψ	$\boldsymbol{\phi}$	ξ	$\psi_{\mathcal{S}}$	ϕ^{α}_{τ}	$\xi_{\mathcal{S}}$
entropy	ρs	$\mathbf{q}/T$	$\zeta \geq 0$	$s_{\mathcal{S}}$	$\mathbf{q}^{\alpha}_{\tau}/T_{\mathcal{S}}$	$\zeta_{\mathcal{S}} \geq 0$

$$\frac{\partial}{\partial t}(\rho s) + \nabla_x \cdot \left(\rho s \mathbf{v} + \frac{\mathbf{q}}{T}\right) = \zeta \geq 0, \tag{2.35}$$

$$\mathring{s}_{\mathcal{S}} + s_{\mathcal{S}} \left(\nabla_{\alpha} w^{\alpha}_{\tau} - 2K_M w_{\nu}\right) + \nabla_{\alpha} \left(\frac{\mathbf{q}^{\alpha}_{\tau}}{T_{\mathcal{S}}}\right) = w_{\nu} \left[\!\left[\rho s\right]\!\right] - \left[\!\left[\rho s \mathbf{v} + \frac{\mathbf{q}}{T}\right]\!\right] \cdot \boldsymbol{\nu} + \zeta_{\mathcal{S}}$$

$$\Leftrightarrow$$

$$\mathring{s}_{\mathcal{S}} + s_{\mathcal{S}} \left(\nabla_{\alpha} w^{\alpha}_{\tau} - 2K_M w_{\nu}\right) + \nabla_{\alpha} \left(\frac{\mathbf{q}^{\alpha}_{\tau}}{T_{\mathcal{S}}}\right) + \left[\!\left[\dot{m} s\right]\!\right] + \left[\!\left[\frac{\mathbf{q}}{T}\right]\!\right] \cdot \boldsymbol{\nu} = \zeta_{\mathcal{S}} \geq 0. \tag{2.36}$$

In the following we want to derive relations for the surface quantity from the entropy principle analogue to those for the bulk phase. So far we assumed that there exists a surface entropy which satisfies (2.36). Now we want to exploit the relations to the other surface quantities. Therefore we assume the surface entropy density to depend on the surface density, the surface temperature and the metric of the surface to respect the geometry, i.e. $s_{\mathcal{S}} = s_{\mathcal{S}}(\rho_{\mathcal{S}}, T_{\mathcal{S}}, g_{\alpha\beta})$. Along with the entropy the surface internal energy $e_{\mathcal{S}}$ also depends on the same set of variables [7]. Depending on the considered problem there may be further variables such as the change of the surface temperature [8]. For the following we want to summarize the assumptions

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[7] This assumption is based on the *principle of equipresence*, see for example [64, 79]

[8] A further important restriction on the constitutive equations and the independent variables comes from the assumption of *material frame indifference*, see [11, 64]. We omit the discussion here and refer to the afore mentioned literature.

(i) We assume the interface to have a uniform temperature (not $[\![T]\!] = 0$) and thus $\nabla_\alpha T_\mathcal{S} = 0$.

(ii) The surface stress only depends on the symmetric tangential component, i.e. $\mathbf{t}_\mathcal{S}^{i\alpha} = S^{\alpha\beta}\boldsymbol{\tau}_\beta$ with $S^{\alpha\beta} = S^{\beta\alpha}$.

(iii) The density of the surface free energy is the coefficient of the surface tension $f_\mathcal{S} = \sigma$, see $(1.66)_1$

(iv) We only consider a single substance and thus the Gibbs energy of the surface $g_\mathcal{S}$ is considered instead of the chemical potential.

To obtain the relations we introduce Lagrange multipliers Λ which may depend on the same variables as the entropy. To ensure the inequality to hold, certain terms have to cancel out[9]. From this requirement we obtain our relations. We yield (applying summation over the space index i)

$$
\begin{aligned}
0 \le \zeta_\mathcal{S} = {} & \mathring{s}_\mathcal{S} + s_\mathcal{S}\left(\nabla_\alpha w_\tau^\alpha - 2K_M w_\nu\right) + \nabla_\alpha\left(\frac{\mathbf{q}_\tau^\alpha}{T_\mathcal{S}}\right) + [\![\dot{m} s]\!] + \left[\!\!\left[\frac{\mathbf{q}}{T}\right]\!\!\right]\cdot\boldsymbol{\nu} \\
& - \Lambda_{\rho_\mathcal{S}}\left(\mathring{\rho}_\mathcal{S} + \rho_\mathcal{S}\left(\nabla_\alpha w_\tau^\alpha - 2K_M w_\nu\right) + [\![\dot{m}]\!]\right) \\
& - \Lambda_{\mathbf{w}_i}\left(\rho_\mathcal{S}\mathring{\mathbf{w}}_i - \nabla_\alpha \mathbf{t}_\mathcal{S}^{i\alpha} + [\![\dot{m}(\mathbf{v}_i - \mathbf{w}_i)]\!] + [\![p]\!]\,\boldsymbol{\nu}_i\right) \\
& - \Lambda_{e_\mathcal{S}}\Bigg(\mathring{e}_\mathcal{S} + \frac{\rho_\mathcal{S}}{2}\mathring{\mathbf{w}}^2 + e_\mathcal{S}\left(\nabla_\alpha w_\tau^\alpha - 2K_M w_\nu\right) + \nabla_\alpha\left(\mathbf{q}_\tau^\alpha - \mathbf{t}_\mathcal{S}^{i\alpha}\mathbf{w}_i\right) \\
& + \left[\!\!\left[\dot{m}\left(e + \frac{\mathbf{v}^2 - \mathbf{w}^2}{2}\right)\right]\!\!\right] + [\![\mathbf{q} + p\mathbf{v}]\!]\cdot\boldsymbol{\nu}\Bigg) \\
= {} & \left(\mathring{s}_\mathcal{S} - \Lambda_{\rho_\mathcal{S}}\mathring{\rho}_\mathcal{S} - \Lambda_{e_\mathcal{S}}\mathring{e}_\mathcal{S} - \left(\Lambda_{\mathbf{w}_i} + \Lambda_{e_\mathcal{S}}\mathbf{w}_i\right)\rho_\mathcal{S}\mathring{\mathbf{w}}_i\right) \\
& + \left(s_\mathcal{S} - \Lambda_{\rho_\mathcal{S}}\rho_\mathcal{S} - \Lambda_{e_\mathcal{S}}e_\mathcal{S}\right)\left(\nabla_\alpha w_\tau^\alpha - 2K_M w_\nu\right) + \Lambda_{\mathbf{w}_i}\nabla_\alpha \mathbf{t}_\mathcal{S}^{i\alpha} + \Lambda_{e_\mathcal{S}}\nabla_\alpha\left(\mathbf{t}_\mathcal{S}^{i\alpha}\mathbf{w}_i\right) \\
& + \nabla_\alpha\left(\frac{\mathbf{q}_\tau^\alpha}{T_\mathcal{S}}\right) - \Lambda_{e_\mathcal{S}}\nabla_\alpha \mathbf{q}_\tau^\alpha \\
& + \left[\!\left[\dot{m}\left(s - \Lambda_{\rho_\mathcal{S}} - \Lambda_{e_\mathcal{S}}e\right)\right]\!\right] - \left[\!\left[p\left(\Lambda_{e_\mathcal{S}}\mathbf{v}\cdot\boldsymbol{\nu} + \Lambda_{\mathbf{w}_i}\boldsymbol{\nu}_i\right)\right]\!\right] - \frac{1}{2}\Lambda_{e_\mathcal{S}}\left[\!\left[\dot{m}\left(\mathbf{v}^2 - \mathbf{w}^2\right)\right]\!\right] \\
& + \left[\!\!\left[\left(\frac{1}{T} - \Lambda_{e_\mathcal{S}}\right)\mathbf{q}\right]\!\!\right]\cdot\boldsymbol{\nu} - \Lambda_{\mathbf{w}_i}[\![\dot{m}\left(\mathbf{v}_i - \mathbf{w}_i\right)]\!]
\end{aligned}
$$

---

[9] In particular for the case with $\dot{m} = 0$ one notices that the inequality is easily violated otherwise.

Now we apply the chain rule to $s_{\mathcal{S}} = s_{\mathcal{S}}(\rho_{\mathcal{S}}, T_{\mathcal{S}}, g_{\alpha\beta})$ and obtain (with (8.23))

$$\begin{aligned}
0 \leq \zeta_{\mathcal{S}} = & \\
& \underbrace{\left(\left(\frac{\partial s_{\mathcal{S}}}{\partial \rho_{\mathcal{S}}} - \Lambda_{\rho_{\mathcal{S}}} - \Lambda_{e_{\mathcal{S}}}\frac{\partial s_{\mathcal{S}}}{\partial \rho_{\mathcal{S}}}\right)\mathring{\rho}_{\mathcal{S}} + \left(\frac{\partial s_{\mathcal{S}}}{\partial T_{\mathcal{S}}} - \Lambda_{e_{\mathcal{S}}}\frac{\partial e_{\mathcal{S}}}{\partial T_{\mathcal{S}}}\right)\mathring{T}_{\mathcal{S}} - \left(\Lambda_{\mathbf{w}_i} + \Lambda_{e_{\mathcal{S}}}\mathbf{w}_i\right)\rho_{\mathcal{S}}\mathring{\mathbf{w}}_i\right)}_{\textbf{(I)}} \\
& \underbrace{\begin{aligned} &+ \left(s_{\mathcal{S}} - \Lambda_{\rho_{\mathcal{S}}}\rho_{\mathcal{S}} - \Lambda_{e_{\mathcal{S}}}e_{\mathcal{S}}\right)\frac{g^{\alpha\beta}}{2}\frac{\partial}{\partial t}g_{\alpha\beta} + \Lambda_{\mathbf{w}_i}\nabla_\alpha \mathbf{t}^{i\alpha}_{\mathcal{S}} + \Lambda_{e_{\mathcal{S}}}\nabla_\alpha\left(\mathbf{t}^{i\alpha}_{\mathcal{S}}\mathbf{w}_i\right) \\ &+ \left(\frac{\partial s_{\mathcal{S}}}{\partial g_{\alpha\beta}} - \Lambda_{e_{\mathcal{S}}}\frac{\partial e_{\mathcal{S}}}{\partial g_{\alpha\beta}}\right)\frac{\partial}{\partial t}g_{\alpha\beta}\end{aligned}}_{\textbf{(II)}} \\
& + \nabla_\alpha\left(\frac{\mathbf{q}^\alpha_\tau}{T_{\mathcal{S}}}\right) - \Lambda_{e_{\mathcal{S}}}\nabla_\alpha \mathbf{q}^\alpha_\tau \\
& + \left\llbracket \dot{m}\left(s - \Lambda_{\rho_{\mathcal{S}}} - \Lambda_{e_{\mathcal{S}}}e\right)\right\rrbracket - \left\llbracket p\left(\Lambda_{e_{\mathcal{S}}}\mathbf{v}\cdot\boldsymbol{\nu} + \Lambda_{\mathbf{w}_i}\boldsymbol{\nu}_i\right)\right\rrbracket - \frac{1}{2}\Lambda_{e_{\mathcal{S}}}\left\llbracket \dot{m}\left(\mathbf{v}^2 - \mathbf{w}^2\right)\right\rrbracket \\
& + \left\llbracket\left(\frac{1}{T} - \Lambda_{e_{\mathcal{S}}}\right)\mathbf{q}\right\rrbracket\cdot\boldsymbol{\nu} - \Lambda_{\mathbf{w}_i}\llbracket \dot{m}\left(\mathbf{v}_i - \mathbf{w}_i\right)\rrbracket . \qquad (2.37)
\end{aligned}$$

Since we want the entropy inequality to be independent of the material time derivatives we obtain for (**I**) the following conditions

$$0 = \frac{\partial s_{\mathcal{S}}}{\partial \rho_{\mathcal{S}}} - \Lambda_{\rho_{\mathcal{S}}} - \Lambda_{e_{\mathcal{S}}}\frac{\partial e_{\mathcal{S}}}{\partial \rho_{\mathcal{S}}}, \qquad (2.38)$$

$$0 = \frac{\partial s_{\mathcal{S}}}{\partial T_{\mathcal{S}}} - \Lambda_{e_{\mathcal{S}}}\frac{\partial e_{\mathcal{S}}}{\partial T_{\mathcal{S}}}, \qquad (2.39)$$

$$0 = \Lambda_{\mathbf{w}_i} + \Lambda_{e_{\mathcal{S}}}\mathbf{w}_i, \qquad (2.40)$$

Using $\mathbf{t}^{i\alpha}_{\mathcal{S}} = S^{\alpha\beta}\boldsymbol{\tau}^i_\beta$ with $S^{\alpha\beta} = S^{\beta\alpha}$ we obtain

$$\mathbf{t}^{i\alpha}_{\mathcal{S}}\nabla_\alpha \mathbf{w}_i = S^{\alpha\beta}\boldsymbol{\tau}_\beta\cdot\nabla_\alpha\mathbf{w} \overset{8.25}{=} \frac{1}{2}S^{\alpha\beta}\frac{\partial}{\partial t}g_{\alpha\beta}.$$

With this we manipulate (**II**) and yield

$$\begin{aligned}
&\left(s_{\mathcal{S}} - \Lambda_{\rho_{\mathcal{S}}}\rho_{\mathcal{S}} - \Lambda_{e_{\mathcal{S}}}e_{\mathcal{S}}\right)\frac{1}{2}g^{\alpha\beta}\frac{\partial}{\partial t}g_{\alpha\beta} + \Lambda_{\mathbf{w}_i}\nabla_\alpha \mathbf{t}^{i\alpha}_{\mathcal{S}} + \Lambda_{e_{\mathcal{S}}}\nabla_\alpha\left(\mathbf{t}^{i\alpha}_{\mathcal{S}}\mathbf{w}_i\right)\\
&+\left(\frac{\partial s_{\mathcal{S}}}{\partial g_{\alpha\beta}} - \Lambda_{e_{\mathcal{S}}}\frac{\partial e_{\mathcal{S}}}{\partial g_{\alpha\beta}}\right)\frac{\partial}{\partial t}g_{\alpha\beta}\\
&=\left(\frac{\partial s_{\mathcal{S}}}{\partial g_{\alpha\beta}} - \Lambda_{e_{\mathcal{S}}}\frac{\partial e_{\mathcal{S}}}{\partial g_{\alpha\beta}} + \frac{1}{2}\Lambda_{e_{\mathcal{S}}}S^{\alpha\beta} + \frac{1}{2}g^{\alpha\beta}\left(s_{\mathcal{S}} - \Lambda_{\rho_{\mathcal{S}}}\rho_{\mathcal{S}} - \Lambda_{e_{\mathcal{S}}}e_{\mathcal{S}}\right)\right)\frac{\partial}{\partial t}g_{\alpha\beta}\\
&+\left(\Lambda_{\mathbf{w}_i} + \Lambda_{e_{\mathcal{S}}}\mathbf{w}_i\right)\nabla_\alpha\mathbf{t}^{i\alpha}_{\mathcal{S}}.
\end{aligned}$$

Thus we further obtain using (2.40)

$$0 = \frac{\partial s_{\mathcal{S}}}{\partial g_{\alpha\beta}} - \Lambda_{e_{\mathcal{S}}}\frac{\partial e_{\mathcal{S}}}{\partial g_{\alpha\beta}} + \frac{1}{2}\Lambda_{e_{\mathcal{S}}}S^{\alpha\beta} + \frac{1}{2}g^{\alpha\beta}\left(s_{\mathcal{S}} - \Lambda_{\rho_{\mathcal{S}}}\rho_{\mathcal{S}} - \Lambda_{e_{\mathcal{S}}}e_{\mathcal{S}}\right). \tag{2.41}$$

To specify the precise values of the Lagrange multipliers we consider (2.37) together with the conditions (2.38) - (2.41). Further we will use the Gibbs energy for the balanced quantities in the bulk phases (compare (1.18)), i.e.

$$g = e - Ts + \frac{p}{\rho}.$$

Altogether we obtain

$$\begin{aligned}
0 \leq \zeta_{\mathcal{S}} &= \nabla_\alpha\left(\frac{\mathbf{q}^\alpha_\tau}{T_{\mathcal{S}}}\right) - \Lambda_{e_{\mathcal{S}}}\nabla_\alpha\mathbf{q}^\alpha_\tau + \left\llbracket \dot{m}\left(s - \Lambda_{\rho_{\mathcal{S}}} - \Lambda_{e_{\mathcal{S}}}e\right)\right\rrbracket - \left\llbracket p\left(\Lambda_{e_{\mathcal{S}}}\mathbf{v}\cdot\boldsymbol{\nu} + \Lambda_{\mathbf{w}_i}\boldsymbol{\nu}_i\right)\right\rrbracket\\
&- \frac{1}{2}\Lambda_{e_{\mathcal{S}}}\left\llbracket \dot{m}\left(\mathbf{v}^2 - \mathbf{w}^2\right)\right\rrbracket + \left\llbracket\left(\frac{1}{T} - \Lambda_{e_{\mathcal{S}}}\right)\mathbf{q}\right\rrbracket\cdot\boldsymbol{\nu} - \Lambda_{\mathbf{w}_i}\left\llbracket \dot{m}\left(\mathbf{v}_i - \mathbf{w}_i\right)\right\rrbracket\\
&= \nabla_\alpha\left(\frac{\mathbf{q}^\alpha_\tau}{T_{\mathcal{S}}}\right) - \Lambda_{e_{\mathcal{S}}}\nabla_\alpha\mathbf{q}^\alpha_\tau\\
&+ \left\llbracket \dot{m}\left(s\left(1 - T\Lambda_{e_{\mathcal{S}}}\right) - \Lambda_{\rho_{\mathcal{S}}} + \frac{g}{T} - \frac{g}{T} - \Lambda_{e_{\mathcal{S}}}\left(e - Ts + \frac{p}{\rho}\right)\right)\right\rrbracket\\
&- \frac{1}{2}\Lambda_{e_{\mathcal{S}}}\left\llbracket \dot{m}\left(\mathbf{v} - \mathbf{w}\right)^2\right\rrbracket + \left\llbracket\left(\frac{1}{T} - \Lambda_{e_{\mathcal{S}}}\right)\mathbf{q}\right\rrbracket\cdot\boldsymbol{\nu}\\
&= \nabla_\alpha\left(\frac{\mathbf{q}^\alpha_\tau}{T_{\mathcal{S}}}\right) - \Lambda_{e_{\mathcal{S}}}\nabla_\alpha\mathbf{q}^\alpha_\tau + \left\llbracket \dot{m}\left(-\Lambda_{\rho_{\mathcal{S}}} - \frac{g}{T}\right) - \frac{1}{2}\Lambda_{e_{\mathcal{S}}}\dot{m}\left(\mathbf{v} - \mathbf{w}\right)^2\right\rrbracket\\
&+ \left\llbracket\left(\frac{1}{T} - \Lambda_{e_{\mathcal{S}}}\right)\left(\mathbf{q}\cdot\boldsymbol{\nu} + \dot{m}\left(g + Ts\right)\right)\right\rrbracket.
\end{aligned} \tag{2.42}$$

Now we consider an equilibrium state and in view of (1.54) and (1.55) we assume the Gibbs energy and the temperature to be continuous across the interface [10]. In particular we expect the surface quantities to coincide with the corresponding bulk quantities. Therefore we choose

$$\Lambda_{e_S} := \frac{1}{T_S}, \; \Lambda_{\rho_S} := -\frac{g_S}{T_S} \quad \text{and thus} \quad \Lambda_{\mathbf{w}_i} = -\frac{\mathbf{w}_i}{T_S}. \tag{2.43}$$

With this choice and $\nabla_\alpha T_S = 0$ equation (2.42) becomes

$$0 \leq \zeta_S = \left[\!\left[\dot{m}\left(\frac{g_S}{T_S} - \frac{g}{T}\right) - \frac{1}{2T_S}\dot{m}\left(\mathbf{v} - \mathbf{w}\right)^2 \right]\!\right] + \left[\!\left[\left(\frac{1}{T} - \frac{1}{T_S}\right)\left(\mathbf{q}\cdot\boldsymbol{\nu} + \dot{m}\left(g + Ts\right)\right) \right]\!\right]. \tag{2.44}$$

Equation (2.39) contains a condition which we already derived in another context, namely $(1.66)_2$. We have with $f_S \equiv \sigma$ and $(2.43)_1$

$$\begin{aligned} 0 &= \frac{\partial s_S}{\partial T_S} - \Lambda_{e_S}\frac{\partial e_S}{\partial T_S} = -\frac{1}{T_S}\left(\frac{\partial e_S}{\partial T_S} - T_S\frac{\partial s_S}{\partial T_S}\right) = -\frac{1}{T_S}\left(s_S + \frac{\partial}{\partial T_S}\left(e_S - T_S s_S\right)\right) \\ &\Leftrightarrow \\ s_S &= -\frac{\partial \sigma}{\partial T_S}. \end{aligned} \tag{2.45}$$

Further we can now also discuss (2.41). Using $f_S \equiv \sigma$ we can write

$$\begin{aligned} 0 &= \frac{\partial s_S}{\partial g_{\alpha\beta}} - \Lambda_{e_S}\frac{\partial e_S}{\partial g_{\alpha\beta}} + \frac{1}{2}\Lambda_{e_S}S^{\alpha\beta} + \frac{1}{2}g^{\alpha\beta}\left(s_S - \Lambda_{\rho_S}\rho_S - \Lambda_{e_S}e_S\right) \\ &= -\frac{1}{T_S}\frac{\partial}{\partial g_{\alpha\beta}}\left(e_S - T_S s_S\right) + \frac{1}{2T_S}S^{\alpha\beta} + \frac{1}{2}\frac{\rho_S g_S}{T_S}g^{\alpha\beta} - \frac{1}{2T_S}g^{\alpha\beta}\left(e_S - T_S s_S\right) \\ &= -\frac{1}{T_S}\frac{\partial \sigma}{\partial g_{\alpha\beta}} + \frac{1}{2T_S}S^{\alpha\beta} + \frac{1}{2T_S}g^{\alpha\beta}\left(\rho_S g_S - \sigma\right). \end{aligned}$$

From this we obtain for $S^{\alpha\beta}$

$$S^{\alpha\beta} = \left(\sigma - \rho_S g_S\right)g^{\alpha\beta} + 2\frac{\partial \sigma}{\partial g_{\alpha\beta}}. \tag{2.46}$$

---

[10] We again refer to [64] for more detailed remarks.

Remark 2.2.1 (Choice of Kinetic Relation). *Later in this work we need an additional equation that determines the mass flux in order to solve the system at hand, see for example Chapter 3. Such an equation is called* kinetic relation *and it has to satisfy the entropy inequality of course. Therefore we distinguish the following cases. Consider an inequality of the form*

$$[\![AB]\!] \geq 0. \tag{2.47}$$

and we are looking for an additional equation for the quantity A. *First we assume* $[\![A]\!] = 0$ *and hence* (2.47) *becomes* $A\,[\![B]\!] \geq 0$. *This inequality is satisfied if* A *is given as a (monotone) function of the form*

$$A = f([\![B]\!]) \begin{cases} > 0, \ [\![B]\!] > 0 \\ = 0, \ [\![B]\!] = 0 \ . \\ < 0, \ [\![B]\!] < 0 \end{cases}$$

A possible simple choice could be the linear ansatz $A = \tau\,[\![B]\!]$ *with* $0 < \tau \in \mathbb{R}$. *Nevertheless several nonlinear choices are possible, e.g.*

$$\begin{aligned} A &= \tau\,[\![B]\!]^p\,, \ 0 < \tau \in \mathbb{R}, \ p = 2k+1, \ k \in \mathbb{N} \\ A &= \tau \sinh\left([\![B]\!]\right), \ 0 < \tau \in \mathbb{R}. \end{aligned}$$

For the second case we assume $[\![A]\!] \neq 0$. *Now we need two kinetic relations. This can be seen as follows*

$$0 \leq [\![AB]\!] = A_2B_2 - A_1B_1.$$

A possible choice in this case could be $A_2 = \alpha B_2$ *with* $0 < \alpha \in \mathbb{R}$ *and* $A_1 = -\beta B_1$ *with* $0 < \beta \in \mathbb{R}$. *This gives*

$$0 \leq [\![AB]\!] = \alpha B_2^2 + \beta B_1^2.$$

These results can be applied to the mass flux by considering $A = \dot{m}$. *Then the first case corresponds to a continuous mass flux across a discontinuity. Whereas the second case corresponds to situation where a surface density of the discontinuity is present.*

2.2.5 Summary

Before we proceed, we briefly want to summarize the obtained local equations for points in the regular phase and on the singular surface, respectively.

Recall, that in order to derive this equations several assumptions had to be made. We consider a single substance and neglect chemical reactions. The fluids are non-viscous and the interface behaves more like a membrane rather than a shell. Further we ignore physical effects induced by electromagnetism, gravitation or radiation. In general the balance laws are given by (2.13) and (2.14)

$$\begin{aligned} \frac{\partial}{\partial t}\psi + \nabla_x \cdot (\psi \mathbf{v} + \boldsymbol{\phi}) &= \xi, \\ \mathring{\psi}_{\mathcal{S}} + \psi_{\mathcal{S}} \left(\nabla_\alpha w_\tau^\alpha - 2K_M w_\nu\right) + \nabla_\alpha \phi_\tau^\alpha &= w_\nu [\![\psi]\!] - [\![\psi \mathbf{v} + \boldsymbol{\phi}]\!] \cdot \boldsymbol{\nu} + \xi_{\mathcal{S}}. \end{aligned}$$

In order to obtain the conservation laws for mass, momentum, energy and the balance law for the entropy we made the following choices for the variables, see Table 2.1. Thus the local equations in the bulk phases are

Ψ	ψ	$\boldsymbol{\phi}$	ξ	$\psi_{\mathcal{S}}$	ϕ_τ^α	$\xi_{\mathcal{S}}$
mass	ρ	0	0	$\rho_{\mathcal{S}}$	0	0
momentum	$\rho \mathbf{v}_i$	$p\mathbf{e}^{(\mathbf{i})}$	0	$\rho_{\mathcal{S}} \mathbf{w}_i$	$-S^{\alpha\beta} \boldsymbol{\tau}_\beta^i$	0
total energy	$\mathcal{E}$	$\mathbf{q} + p\mathbf{v}$	0	$\mathcal{E}_{\mathcal{S}}$	$\mathbf{q}_\tau^\alpha - S^{\alpha\beta} \boldsymbol{\tau}_\beta \cdot \mathbf{w}$	0
entropy	ρs	$\mathbf{q}/T$	ζ	$s_{\mathcal{S}}$	$\mathbf{q}_\tau^\alpha / T_{\mathcal{S}}$	$\zeta_{\mathcal{S}}$

Table 2.1: Summary of the different variable choices according to the considered quantity Ψ.

given by

$$\begin{aligned} \frac{\partial}{\partial t}\rho + \nabla_x \cdot (\rho \mathbf{v}) &= 0, \\ \frac{\partial}{\partial t}(\rho \mathbf{v}_i) + \nabla_x \cdot \left(\rho \mathbf{v}_i \mathbf{v} + p\mathbf{e}^{(\mathbf{i})}\right) &= 0, \ i \in \{1,2,3\}, \\ \frac{\partial}{\partial t}\mathcal{E} + \nabla_x \cdot (\mathbf{v}(\mathcal{E} + p) + \mathbf{q}) &= 0, \\ \frac{\partial}{\partial t}(\rho s) + \nabla_x \cdot \left(\rho s \mathbf{v} + \frac{\mathbf{q}}{T}\right) &= \zeta \geq 0. \end{aligned}$$

The surface equations are

$$\begin{aligned}
&\mathring{\rho}_{\mathcal{S}} + \rho_{\mathcal{S}} \left(\nabla_\alpha w_\tau^\alpha - 2K_M w_\nu\right) = -[\![\dot{m}]\!]\,,\\
&\rho_{\mathcal{S}} \mathring{\mathbf{w}}_i - \nabla_\alpha \mathbf{t}_{\mathcal{S}}^{i\alpha} = -[\![\dot{m}(\mathbf{v}_i - \mathbf{w}_i)]\!] - [\![p]\!]\,\boldsymbol{\nu}_i,\;\; i \in \{1,2,3\},\\
&\mathring{e}_{\mathcal{S}} + \frac{\rho_{\mathcal{S}}}{2}(\mathring{\mathbf{w}}^2) + e_{\mathcal{S}} \left(\nabla_\alpha w_\tau^\alpha - 2K_M w_\nu\right) + \nabla_\alpha \left(\mathbf{q}_\tau^\alpha - \mathbf{t}_{\mathcal{S}}^{i\alpha}\mathbf{w}_i\right)\\
&= -\left[\!\!\left[\dot{m}\left(e + \frac{\mathbf{v}^2 - \mathbf{w}^2}{2}\right)\right]\!\!\right] - [\![\mathbf{q} + p\mathbf{v}]\!] \cdot \boldsymbol{\nu}\\
&\mathring{s}_{\mathcal{S}} + s_{\mathcal{S}} \left(\nabla_\alpha w_\tau^\alpha - 2K_M w_\nu\right) + \nabla_\alpha \left(\frac{\mathbf{q}_\tau^\alpha}{T_{\mathcal{S}}}\right) + [\![\dot{m}s]\!] + \left[\!\!\left[\frac{\mathbf{q}}{T}\right]\!\!\right] \cdot \boldsymbol{\nu} = \zeta_{\mathcal{S}} \geq 0.
\end{aligned}$$

The surface entropy is a function of the surface density, surface temperature and the metric. We derived explicit conditions to assure compatibility with thermodynamics, i.e.

$$s_{\mathcal{S}} = -\frac{\partial \sigma}{\partial T_{\mathcal{S}}} \quad \text{and} \quad S^{\alpha\beta} = \left(\sigma - \rho_{\mathcal{S}} g_{\mathcal{S}}\right) g^{\alpha\beta} + 2\frac{\partial \sigma}{\partial g_{\alpha\beta}}.$$

Further the entropy inequality may be written as

$$0 \leq \zeta_{\mathcal{S}} = \left[\!\!\left[\dot{m}\left(\frac{g_{\mathcal{S}}}{T_{\mathcal{S}}} - \frac{g}{T}\right) - \frac{1}{2T_{\mathcal{S}}}\dot{m}\left(\mathbf{v} - \mathbf{w}\right)^2\right]\!\!\right] + \left[\!\!\left[\left(\frac{1}{T} - \frac{1}{T_{\mathcal{S}}}\right)\left(\mathbf{q}\cdot\boldsymbol{\nu} + \dot{m}\left(g + Ts\right)\right)\right]\!\!\right].$$

and thus the lower dimensional cases are immediately obvious. As an exemplary application of the above results for singular surfaces we want to derive the *Young-Laplace Law*. Therefore we assume a spherical surface with radius R when there is no mass flux across the interface. Further we assume $\rho_{\mathcal{S}} \equiv 0$ and that the surface free energy density does not depend on the metric. With these assumptions we obtain for the surface stress using (2.46) and (8.14)

$$S^{\alpha\beta} = \sigma(T_{\mathcal{S}})g^{\alpha\beta} \quad \text{and} \quad \nabla_\alpha \mathbf{t}_{\mathcal{S}}^{i\alpha} = S^{\alpha\beta} b_{\alpha\beta} \boldsymbol{\nu}^i = 2\frac{\sigma}{R}\boldsymbol{\nu}^i.$$

Then (2.23) reduces to the well known *Young-Laplace Law*

$$[\![p]\!] = 2\sigma K_M = 2\frac{\sigma}{R}. \tag{2.48}$$

2.3 Results for Hyperbolic Conservation Laws

The results in the previous sections where mostly driven by physical arguments. Thus we said nothing about the mathematical structure of the obtained equations in Section 2.2. Throughout this work we will consider the Euler equations which form a system of hyperbolic conservation laws. Therefore we want to give a brief introduction into the mathematics of hyperbolic conservation laws. As mentioned before we recommend the books of Dafermos [18], Evans [28], LeFloch [55], Smoller [75] and Warnecke [85] for further reading. Concerning the Euler equations we also refer to the works of Chen [15, 16]. The afore mentioned literature also contains many useful references for the various aspects of problems related to (hyperbolic) balance laws.

Due to the complexity of the topic we just briefly note the most important statements on hyperbolic partial differential equations. The probably most fundamental property of hyperbolic equations is that (any abstract) information is propagated at *finite* speed. This has several consequences, one of the most severe ones is that even for smooth initial data one has to expect discontinuities in finite time. In fact this problem already occurs for single nonlinear equations in one dimension. These difficulties are best understood by investigating one dimensional prototype examples such as the *linear advection equation* or the *Burgers equation*. The phenomena that can be studied with these equations are the transport of the solution along *characteristic curves*, formation of *shocks* and the non-uniqueness of solutions. We omit the details here since these examples are quasi textbook classics and we refer to the literature mentioned above. The case of scalar conservation laws is pretty much understood and one may find all important results in the given literature [11]. This is in contrast to the situation when systems (even in one space dimension) are considered. There the theory is far from being completely understood, again we exemplary refer to the comments in [18] [12]. It is the loss of smoothness from which the difficulties arise. First and foremost it leads to the difficulty of defining an adequate notion of weak solution which allows discontinuities. Along with this the problem of non-uniqueness arises. Therefore mathematicians tried to exploit (mathematical) criteria from physical considerations which then pick the correct solution. Without going into the details these are the *vanishing viscosity ap-*

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[11] To quote Dafermos as in [18] (*p*.145):*"The theory of the scalar balance law, in several spatial dimensions, has reached a state of virtual completeness."*

[12] *"At the present time the theory of multidimensional systems is terra incognita [...]."*, [18] (*p*.195).

proach, the method of *entropy inequalities* and in one space dimension the *Lax condition*. It turns out that (apart from certain exceptions) it is very difficult to establish these criteria for systems in general. Thus general existence and uniqueness results for systems of hyperbolic partial differential equations are still a field of active research. This of course also affects the theory of numerical algorithms, which crucially needs analytical tools to single out the admissible solution. However, in certain special cases this is possible.

We now turn to such a special situation, since our focus is on the Riemann problem for the Euler equations. Hence in the following we consider *systems of hyperbolic conservation laws* [13]. A general system of conservation laws is of the following form

$$\begin{aligned} \frac{\partial}{\partial t}u_1(t,\mathbf{x}) + \nabla_x \cdot F_1(u_1(t,\mathbf{x}),\dots,u_m(t,\mathbf{x})) &= 0, \\ &\vdots \\ \frac{\partial}{\partial t}u_m(t,\mathbf{x}) + \nabla_x \cdot F_m(u_1(t,\mathbf{x}),\dots,u_m(t,\mathbf{x})) &= 0. \end{aligned} \tag{2.49}$$

Here $t \in [0, t_{max}) \subseteq \mathbb{R}_+$ denotes the time variable and the space variable is given by $\mathbf{x} \in \Omega \subseteq \mathbb{R}^n$. The unknowns are denoted by u_i with $u_i : \mathbb{R}\times\mathbb{R}^n \to \mathbb{R}$ and are called *conserved quantities*. The functions $F_i : \mathbb{R}^m \to \mathbb{R}^n$ are the *fluxes*. Introducing $\mathbf{u} = (u_1, \dots, u_m)$ and $\mathbf{F} = (F_1, \dots, F_m)$ we can write (2.49) as

$$\frac{\partial}{\partial t}\mathbf{u}(t,\mathbf{x}) + \nabla_x \cdot \mathbf{F}(\mathbf{u}) = 0. \tag{2.50}$$

Here we understand the divergence in the sense that it is applied to each row of the $m \times n$ matrix $\mathbf{F}(\mathbf{u})$. Usually one refers to the open set $\mathcal{U} \subseteq \mathbb{R}^m$ with $\mathbf{u} \in \mathcal{U}$ as the *state space* or *state domain*.
In the case of one space dimension we have $\mathbf{u} : \mathbb{R}\times\mathbb{R} \to \mathbb{R}^m$ and $\mathbf{F} : \mathbb{R}^m \to \mathbb{R}^m$ and thus write

$$\frac{\partial}{\partial t}\mathbf{u}(t,x) + \frac{\partial}{\partial x}\mathbf{F}(\mathbf{u}) = 0. \tag{2.51}$$

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[13] Be aware that there is a difference in the use of conservation law. For example the balance of momentum (2.64) is a mathematical conservation law, whereas it fails to do so in the sense that the right hand side of (2.1) vanishes.

The first major concept that is introduced to study (2.51) is *hyperbolicity*. [14]. We will use the following notation. The Jacobian of $\mathbf{F} : \mathcal{U} \to \mathbb{R}^m$ is given by

$$\mathbf{DF}(\mathbf{u}) = \begin{pmatrix} \frac{\partial F_1}{\partial u_1} & \cdots & \frac{\partial F_1}{\partial u_m} \\ \vdots & & \vdots \\ \frac{\partial F_m}{\partial u_1} & \cdots & \frac{\partial F_m}{\partial u_m} \end{pmatrix}. \tag{2.52}$$

and the eigenvalues are denoted by $\lambda_1(\mathbf{u}), \dots, \lambda_m(\mathbf{u})$. The right eigenvectors are then given by

$$\mathbf{DF}(\mathbf{u}) \cdot \mathbf{r}_i(\mathbf{u}) = \lambda_i(\mathbf{u})\mathbf{r}_i(\mathbf{u}),\ i \in \{1, \dots, m\}. \tag{2.53}$$

The pair $(\lambda_i(\mathbf{u}), \mathbf{r}_i(\mathbf{u}))$ is called *i-th characteristic field*.

Definition 2.3.1 (Hyperbolicity)**.** *The System (2.51) is called hyperbolic (in (t, x)) if there are m real eigenvalues $\lambda_1(\mathbf{u}), \dots, \lambda_m(\mathbf{u})$, and m corresponding linearly independent eigenvectors $\mathbf{r}_1(\mathbf{u}), \dots, \mathbf{r}_m(\mathbf{u})$, of the Jacobian of the flux function (2.52). If additionally the eigenvalues are all distinct, the system is called strictly hyperbolic. The system (2.51) is called elliptic if none of the eigenvalues is real and otherwise one says that it is of composite type. Systems that are hyperbolic in one region and elliptic in another are said to be of mixed type.*

If not stated otherwise we henceforth assume that the system (2.51) is strictly hyperbolic and we therefore have m linearly independent eigenvectors [15] [16]. It can be shown that hyperbolicity is invariant under coordinate changes with respect to the state space, see [28]. This allows certain reformulations of (2.51) without loosing hyperbolicity. Further it is possible to prove that if the Jacobian is smooth and strictly hyperbolic that the eigenvalues and eigenvectors depend smoothly on $\mathbf{u} \in \mathcal{U}$, see [28].

We already mentioned that scalar conservation laws exhibit phenomena that will also occur in the case of systems. Therefore one seeks to transfer the concepts of scalar conservation laws to the case of systems as it is done

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[14] Here we define hyperbolicity only for one spatial dimension. In fact even in the multidimensional case, hyperbolicity essentially remains one dimensional in the sense that the Jacobian in every direction should be hyperbolic, see [15, 18].

[15] It is shown in [15] and the references therein that in three spatial dimensions there are no strictly hyperbolic systems with $m \equiv 2 \mod 4$.

[16] It is exemplary shown in [12] that if the system is not strictly hyperbolic, the solution may not depend continuously on the initial data.

in the following.
Scalar conservation laws, for the sake of simplicity in one space dimension, are distinguished according to the mathematical nature of the flux function. If the derivative of the flux function is a constant the equation is called linear, see for example the *linear advection equation* with $f(u) = au, a \in \mathbb{R}$. In the case of a nonlinear (strict monotone) flux function the equation is called nonlinear, see for example the *Burgers equation* with $f(u) = u^2/2$. Now the concept of linearity/nonlinearity is extended to the case of systems by investigating the geometrical relation of an eigenvector and the gradient of the corresponding eigenvalue.

Definition 2.3.2 (Genuine Nonlinear/Linearly Degenerated)**.** *The i-th characteristic field* $(\lambda_i(\mathbf{u}), \mathbf{r}_i(\mathbf{u}))$ *of the system (2.51) is called*

(i) genuine nonlinear *if* $\nabla_u \lambda_i(\mathbf{u}) \cdot \mathbf{r}_i(\mathbf{u}) \neq 0$ *for all* $\mathbf{u} \in \mathcal{U}$

(ii) linearly degenerated *if* $\nabla_u \lambda_i(\mathbf{u}) \cdot \mathbf{r}_i(\mathbf{u}) = 0$ *for all* $\mathbf{u} \in \mathcal{U}$.

The operator ∇_u *denotes the gradient with respect to the chosen state variables.*

For a definition in multiple dimensions and further implications, results and literature see for example [15][17]. It is an important observation for the Euler equations that whether a characteristic field is *genuine nonlinear* or not is solely defined by the thermodynamic properties of the considered fluid, cf. [60].
A nice interpretation of the above defined properties can be obtained from the following considerations, cf. [28]. Assume we search for solutions of (2.51) of the type $\mathbf{u}(t,x) = \mathbf{v}(w(t,x))$ with $\mathbf{v} : \mathbb{R} \to \mathbb{R}^m$ and $w : [0,\infty) \times \mathbb{R} \to \mathbb{R}$. The function $\mathbf{v}$ and w have to be determined. These solutions are called *simple waves*. Inserting this ansatz in (2.51) gives

$$\dot{\mathbf{v}}(w)\frac{\partial}{\partial t}w + \mathbf{DF}(\mathbf{v}(w))\dot{\mathbf{v}}(w)\frac{\partial}{\partial x}w = 0. \tag{2.54}$$

It can easily be seen that the system (2.54) holds true if for one $i \in \{1, \ldots, m\}$ and a scalar $c(s) \in \mathbb{R}$ the following equations hold

$$\frac{\partial}{\partial t}w + \lambda_i(\mathbf{v}(w))\frac{\partial}{\partial x}w = 0 \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}s}\mathbf{v}(s) = c(s)\mathbf{r}_i(\mathbf{v}(s)). \tag{2.55}$$

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[17] It is also proven in [15] that in the case of two spatial dimensions and systems of $m = 2k$ equations with $k \geq 1$ being an odd natural number there is always one linearly degenerate eigenvalue.

From (2.55) we can draw two important conclusions. First we see that once the function $\mathbf{v}(s)$ is obtained from the ODE $(2.55)_2$ [18], the equation $(2.55)_1$ may be interpreted as scalar conservation law for w. Second we consider the change of the eigenvalue along the curve $s \mapsto \mathbf{v}(s)$ and obtain using $(2.55)_2$

$$\frac{\mathrm{d}}{\mathrm{d}s}\lambda_i(\mathbf{v}(s)) = \nabla_u \lambda_i(\mathbf{v}(s))\frac{\mathrm{d}}{\mathrm{d}s}\mathbf{v}(s) = \nabla_u \lambda_i(\mathbf{v}(s))\mathbf{r}_i(\mathbf{v}(s)). \tag{2.56}$$

Thus regarding Definition 2.3.2 a genuine nonlinear characteristic field states that the eigenvalue is strictly monotone along the curve $\mathbf{v}(s)$. A linearly degenerated characteristic field states that the eigenvalue is constant along the curve $\mathbf{v}(s)$. This highlights the connection to the scalar equations. Concerning equation $(2.55)_2$ there is another important observation in the case of smooth solutions. Given a smooth solution we may apply a nonlinear transformation of the variables aiming to simplify (2.51) using another appropriate choice of variables. Such a special set of variables is given by the *Riemann invariants*, cf. [18, 28, 75].

Definition 2.3.3. *An i-th Riemann invariant is a smooth function $\boldsymbol{\omega}_i : \boldsymbol{\mathcal{U}} \to \mathbb{R}$ such that*

$$\nabla_u \boldsymbol{\omega}_i(\mathbf{u}) \cdot \mathbf{r}_i(\mathbf{u}) = 0.$$

Note, that in general Riemann invariants do not have to exist. Now the important observation is that an i-th Riemann invariant is constant across a simple wave [19]. To obtain the Riemann invariants one may use $(2.55)_2$, which will be exemplary shown in Section 2.4.

For the above considerations we assumed enough smoothness of the functions in order to perform the calculations. Now we want to turn to the situation in the presence of discontinuities. Thus we need the definition of a *weak solution*. Therefore we consider (2.51) with an initial condition

$$\begin{cases} \dfrac{\partial}{\partial t}\mathbf{u}(t,x) + \dfrac{\partial}{\partial x}\mathbf{F}(\mathbf{u}) & = 0,\ (t,x) \in (0,t_{max}) \times \mathbb{R} \\ \mathbf{u}(0,x) & = \mathbf{u}_0(x),\ x \in \mathbb{R}. \end{cases} \tag{2.57}$$

Now the usual idea is to assume a smooth solution and multiply (2.51) with a smooth test function with compact support. Then one integrate by parts and thus obtains a formulation which needs less regularity than assumed

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[18] The curve $\mathbf{v}(s)$ as given in $(2.55)_2$ is also called *integral curve*, cf. [55].

[19] Indeed, in [75] Riemann invariants are used to define simple waves

and hence can be used to define a weak solution, see for example [18, 28, 75] and [85].

Definition 2.3.4 (Weak Solution)**.** *A function (measurable and bounded)* $\mathbf{u} : (0, t_{max}) \times \mathbb{R} \to \mathbb{R}^m$ *is called weak solution of (2.57) if it solves*

$$\int_0^{t_{max}} \int_{-\infty}^{+\infty} \mathbf{u} \cdot \frac{\partial}{\partial t} \boldsymbol{\varphi} + \mathbf{F}(\mathbf{u}) \cdot \frac{\partial}{\partial x} \boldsymbol{\varphi} \, \mathrm{d}x\mathrm{d}t + \int_{-\infty}^{+\infty} \mathbf{u}(0, x) \cdot \boldsymbol{\varphi}(0, x) \, \mathrm{d}x = 0 \tag{2.58}$$

for every test function $\boldsymbol{\varphi} \in \left[C_0^\infty([0, t_{max}) \times \mathbb{R}) \right]^m$.

Let us now consider the situation where we have a region $\mathcal{V} \subset (0, t_{max}) \times \mathbb{R}$ which is divided by a smooth curve $\mathcal{S}$ into $\mathcal{V}_1$ and $\mathcal{V}_2$. Further we assume that we have a smooth solution in $\mathcal{V}_1$ and $\mathcal{V}_2$, respectively. Thus in each part the PDE (2.51) holds. Note that in contrast to the situation in Section 2.1 we neglect additional contributions of functions defined on the curve $\mathcal{S}$. Now we choose a test function $\boldsymbol{\varphi}$ with compact support in $\mathcal{V}$ which does not necessarily vanish on $\mathcal{S}$ and use equation (2.58) to obtain

$$\begin{aligned} 0 &= \int_0^{t_{max}} \int_{-\infty}^{+\infty} \mathbf{u} \cdot \frac{\partial}{\partial t} \boldsymbol{\varphi} + \mathbf{F}(\mathbf{u}) \cdot \frac{\partial}{\partial x} \boldsymbol{\varphi} \, \mathrm{d}x\mathrm{d}t \\ &= \int_0^{t_{max}} \int_{\mathcal{V}_1} \mathbf{u} \cdot \frac{\partial}{\partial t} \boldsymbol{\varphi} + \mathbf{F}(\mathbf{u}) \cdot \frac{\partial}{\partial x} \boldsymbol{\varphi} \, \mathrm{d}x\mathrm{d}t + \int_0^{t_{max}} \int_{\mathcal{V}_2} \mathbf{u} \cdot \frac{\partial}{\partial t} \boldsymbol{\varphi} + \mathbf{F}(\mathbf{u}) \cdot \frac{\partial}{\partial x} \boldsymbol{\varphi} \, \mathrm{d}x\mathrm{d}t. \end{aligned}$$

Since $\boldsymbol{\varphi}$ has compact support in $\mathcal{V}$ we derive

$$\begin{aligned} \int_0^{t_{max}} \int_{\mathcal{V}_1} \mathbf{u} \cdot \frac{\partial}{\partial t} \boldsymbol{\varphi} + \mathbf{F}(\mathbf{u}) \cdot \frac{\partial}{\partial x} \boldsymbol{\varphi} \, \mathrm{d}x\mathrm{d}t &= - \int_0^{t_{max}} \int_{\mathcal{V}_1} \left(\frac{\partial}{\partial t} \mathbf{u} + \frac{\partial}{\partial x} \mathbf{F}(\mathbf{u}) \right) \cdot \boldsymbol{\varphi} \, \mathrm{d}x\mathrm{d}t \\ &\quad + \int_{\mathcal{S}} \left(\mathbf{u}_1 \nu^{(1)} + \mathbf{F}(\mathbf{u}_1) \nu^{(2)} \right) \cdot \boldsymbol{\varphi} \, \mathrm{d}l \\ &= \int_{\mathcal{S}} \left(\mathbf{u}_1 \nu^{(1)} + \mathbf{F}(\mathbf{u}_1) \nu^{(2)} \right) \cdot \boldsymbol{\varphi} \, \mathrm{d}l. \end{aligned}$$

Here $\boldsymbol{\nu} = (\nu^{(1)}, \nu^{(2)})$ is the unit normal of $\mathcal{S}$ analogous to the situation in Figure 2.1, Section 2.1. A similar calculation for the right part together with the starting point (2.58) gives

$$0 = \int\limits_{\mathcal{S}} \left[(\mathbf{u}_2 - \mathbf{u}_1)\, \nu^{(1)} + (\mathbf{F}(\mathbf{u}_2) - \mathbf{F}(\mathbf{u}_1))\, \nu^{(2)} \right] \cdot \boldsymbol{\varphi}\, \mathrm{d}l$$

Since this equation should be true for all smooth test functions we demand along $\mathcal{S}$

$$0 = (\mathbf{u}_2 - \mathbf{u}_1)\, \nu^{(1)} + (\mathbf{F}(\mathbf{u}_2) - \mathbf{F}(\mathbf{u}_1))\, \nu^{(2)}.$$

If we now choose a suited parametrization $(t, \gamma(t))$ of $\mathcal{S}$ we may compute the unit normal $\boldsymbol{\nu} = (-\dot{\gamma}, 1)/\sqrt{1 + \dot{\gamma}^2}$. With this we finally obtain the *Rankine-Hugoniot* jump conditions with $S = \dot{\gamma}$ being the speed of $\mathcal{S}$

$$[\![\mathbf{F}(\mathbf{u})]\!] = S\, [\![\mathbf{u}]\!] \,. \tag{2.59}$$

Note that equation (2.59) is a special situation of the more general jump conditions derived in Section 2.1. This can be seen by canceling all surface related terms and neglect the source terms in equation (2.14). Moreover (2.59) is a vector valued equation which has to hold in each component. Further we have that a weak solution of (2.51) has to satisfy the jump conditions (2.59) in the presence of discontinuities.

Now we want to give some details of Riemann problem which we will need later on. For the various details we refer to the literature, e.g. [18, 28, 55, 75] and [85]. The Riemann problem for a system of conservation laws is given by (2.51) together with piecewise constant initial data, i.e.

$$\begin{aligned} \frac{\partial}{\partial t}\mathbf{u} + \frac{\partial}{\partial x}\mathbf{F}(\mathbf{u}) = 0 \text{ with } \mathbf{u} = \mathbf{u}(t,x) \in \mathcal{U} \text{ and } (t,x) \in (0, t_{max}) \times \mathbb{R} \\ \mathbf{u}(0,\mathbf{x}) = \begin{cases} \mathbf{u}_L, \; x < 0 \\ \mathbf{u}_R, \; x > 0 \end{cases} \quad . \end{aligned} \tag{2.60}$$

It is the simplest non-trivial type of problem which solution exhibits all the classical nonlinear phenomena of hyperbolic conservation laws. All quantities are given as before, $\mathcal{U} \subseteq \mathbb{R}^m$ is the state space and the flux is given by a smooth function $\mathbf{F} : \mathcal{U} \to \mathbb{R}^m$. Further we assume that the Jacobian $\mathbf{DF}(\mathbf{u})$ has m distinct real eigenvalues with a corresponding set

of linearly independent eigenvectors. Thus we have a strictly hyperbolic system. Additionally all the characteristic fields are assumed to be either genuine nonlinear or linearly degenerated.
One can immediately verify that the problem (2.60) is invariant under the transformation $(t, x) \mapsto (\alpha t, \alpha x)$ with $\alpha > 0$. Therefore we look for a *self-similar solution* $\mathbf{u}(t, x) = \mathbf{u}(x/t)$. In the following we will use $\xi := x/t$. Considering (2.60) the solution has to satisfy the following conditions (the prime denotes the derivative with respect to ξ)

$$\begin{aligned} -\mathbf{u}'(\xi)\xi + \mathbf{F}(\mathbf{u}(\xi))' &= 0, \\ \mathbf{u}(-\infty) &= \mathbf{u}_L, \\ \mathbf{u}(+\infty) &= \mathbf{u}_R. \end{aligned} \tag{2.61}$$

Concerning the ansatz for the simple waves given before we can already draw important conclusions. In our special situation we have $\mathbf{u}(t, x) = \mathbf{u}(x/t)$ with the function $w(t, x) = \xi$ and thus $(2.55)_1$ reduces to

$$\frac{\partial}{\partial t} w + \lambda_i(\mathbf{u}(w)) \frac{\partial}{\partial x} w = 0 \quad \Leftrightarrow \quad \lambda_i(\mathbf{u}(\xi)) = \xi. \tag{2.62}$$

From equation (2.62) we immediately can see that the characteristic curves $x(t)$ are straight lines, i.e. curves where the solution is constant

$$0 = \frac{\mathrm{d}w}{\mathrm{d}t}(t, x(t)) = \frac{\partial}{\partial t} w + \frac{\mathrm{d}x}{\mathrm{d}t} \frac{\partial}{\partial x} w \quad \text{with} \quad \frac{\mathrm{d}x}{\mathrm{d}t} = \lambda_i(\mathbf{u}(\xi)) = \xi.$$

Now we turn towards the different types of waves that may occur in the solution of the Riemann problem. We can distinguish three different types of waves. Intuitively this can be seen by considering the (straight) characteristics in the $x - t$ plane, see the following Figures 2.3 and 2.5. The first two wave types are associated to genuine nonlinear fields and may be exemplary investigated by studying the Burgers equation.

Rarefaction Wave: First there is the case of diverging characteristic fields, i.e. $\lambda_i(\mathbf{u}_L) < \lambda_i(\mathbf{u}_R)$, see Figure 2.3. In this case we have a smooth solution called *rarefaction wave* and the slope of the characteristics between the left and the right state is given by (2.62), i.e. $\lambda_i(\mathbf{u}(\xi)) = \xi$. The solution can be obtained using $(2.55)_2$ with the normalization $c(s) = (\nabla_u \lambda_i(\mathbf{u}(s)) \mathbf{r}_i(\mathbf{u}(s)))^{-1}$, i.e.

$$\mathbf{u}(\xi)' = c(\xi) \mathbf{r}_i(\mathbf{u}(\xi)),$$

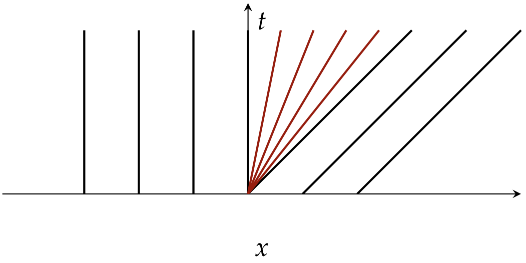

Figure 2.3: Diverging characteristics in the case of a rarefaction wave.

cf. [85]. Sometimes one also refers to system $(2.55)_2$ as the Riemann Invariants, e.g. [78].

Shock Wave: Second we might face the situation where the characteristics intersect and form a shock or at later times run into a shock. In this situation the solution is discontinuous and we have to use the Rankine-Hugoniot condition (2.59)

$$[\![\mathbf{F}(\mathbf{u})]\!] = S_i\,[\![\mathbf{u}]\!]\,.$$

Here S_i denotes the velocity of the i-th shock. For the eigenvalues we have in this situation $\lambda_i(\mathbf{u}_L) > S_i > \lambda_i(\mathbf{u}_R)$ which is exactly the Lax entropy criterion, see Figure 2.4 (a). The Lax entropy criterion ensures uniqueness of the solution in one dimension. Among all possible solutions it singles out the entropy solution in the case that all characteristic fields are either genuine

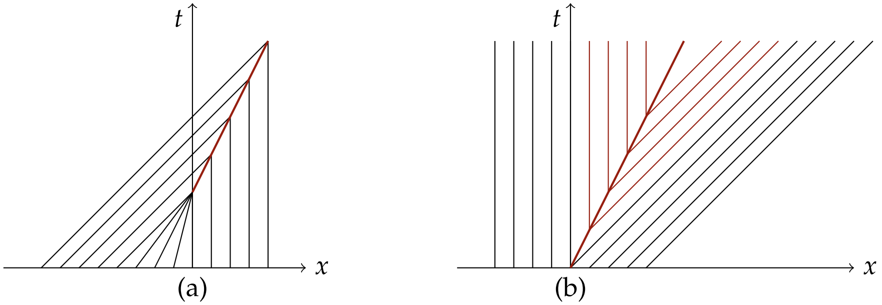

Figure 2.4: Characteristics in the presence of discontinuities.

nonlinear or linearly degenerated. Moreover it rules out the case the characteristics may run out of discontinuities instead of running into them, see Figure 2.4 (b).

Contact Discontinuity: The remaining wave type is associated to a linearly degenerated characteristic field. In this case we have $\lambda_i(\mathbf{u}_L) = \lambda_i(\mathbf{u}_R) = S_i$ due to equation (2.56). Geometrically this means that all characteristics are parallel to each other, see Figure 2.5. Further the Rankine-Hugoniot conditions (2.59) as well as the Riemann Invariants $(2.55)_2$ are fulfilled. In particular the characteristic speeds of the neighbouring characteristics are constant across the wave and coincide with the speed of the contact wave.

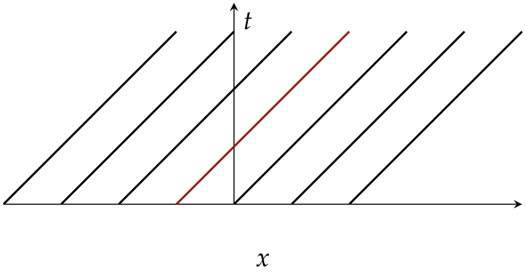

Figure 2.5: Parallel characteristics in the case of a contact discontinuity.

Now the key observation is that a solution to the Riemann problem (2.60) can be constructed by piecing together the different wave types such that the conditions (2.61) as well as the conditions for each wave are satisfied. For the mathematical justification we refer to the literature, e.g. [28, 55, 75]. In the following Section 2.4 we will give more details for the Euler equations since these equations are the main objective of the present work.

2.4 Euler Equations

In Section 2.2 we derived a system of six partial differential equations accompanied by six equations for points on singular surfaces. The aim of this section is to derive three submodels from these equations. These models are obtained by considering different physical processes. A common property of these three systems is that they form a system of hyperbolic conservation laws. All these systems are called Euler equations, which is sometimes a bit misleading. With *the* Euler equation one originally referred to (2.24), see [52]. The *adiabatic Euler equations* are usually referred to as *the* Euler equations or the full Euler system. Quite often the isothermal and isentropic Euler equations are then often thought of as submodels of the Euler equations. We want to emphasize that we prefer the point of view, that all three types of models are submodels of the equations obtained in Section 2.2. This is mainly due to the fact, that it is for example physically arguable to derive the isothermal ($T = const.$) from the adiabatic ($\mathbf{q} \equiv 0$) Euler equations.

2.4.1 Adiabatic Euler Equations

The "classical" system of Euler equations is obtained by assuming a physical system which is *adiabatically* isolated such that $\mathbf{q} \equiv 0$. Thus we also refer to this system as the *adiabatic Euler equations*. Note that this is not equivalent to an *adiabatic process*. An adiabatic process is reversible and implies constant entropy (see [51]), which of course is in general not the case (e.g. due to shock waves). [20] Further we assume that the surface quantities vanish identically, i.e. $\rho_{\mathcal{S}} \equiv 0$ and $e_{\mathcal{S}} \equiv 0$. Additionally we assume that the metric is constant in time, i.e. $\partial_t g_{\alpha\beta} = 0$. Note that in the single phase case the jump conditions only apply to shock waves and hence we then also neglect the surface stress. Otherwise there would be a remaining contribution in the balances for the momentum and for the energy in singular points.
The system of Euler equations is given by

$$\frac{\partial}{\partial t}\rho + \nabla_x \cdot (\rho \mathbf{v}) = 0, \tag{2.63}$$

$$\frac{\partial}{\partial t}(\rho \mathbf{v}^i) + \nabla_x \cdot \left(\rho \mathbf{v}^i \mathbf{v} + p\mathbf{e}^{(\mathbf{i})}\right) = 0, \ i \in \{1,2,3\}, \tag{2.64}$$

$$\frac{\partial}{\partial t}\mathcal{E} + \nabla_x \cdot (\mathbf{v}\,(\mathcal{E} + p)) = 0. \tag{2.65}$$

The corresponding jump conditions across discontinuities are given by

$$[\![\dot{m}]\!] = 0, \tag{2.66}$$

$$\dot{m}\,[\![\mathbf{v}_i]\!] + [\![p]\!]\,\boldsymbol{\nu}_i = 0, \ i \in \{1,2,3\}, \tag{2.67}$$

$$\dot{m}\left[\!\!\left[e + \frac{1}{2}\mathbf{v}^2 + p\mathbf{v}\cdot\boldsymbol{\nu}\right]\!\!\right] = 0. \tag{2.68}$$

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[20] In general one should be careful when the word *adiabatic* is used, since it might have different meanings depending on the context where it is used.

Equation (2.68) can be reformulated using (2.67) and one obtains

$$\dot{m} \left[\!\!\left[e + \frac{p}{\rho} + \frac{1}{2} (\mathbf{v} - \mathbf{w})^2 \right]\!\!\right] = 0. \tag{2.69}$$

The entropy is balanced by the following equations

$$\frac{\partial}{\partial t}(\rho s) + \nabla_x \cdot (\rho s \mathbf{v}) = 0, \tag{2.70}$$

$$\dot{m} [\![s]\!] = \zeta_{\mathcal{S}} \geq 0. \tag{2.71}$$

Note that the entropy is conserved away from discontinuities. That the bulk entropy productions vanishes is due to our assumption of $\mathbf{q} \equiv 0$ and that we neglected other effect such as diffusion, viscosity or chemical reactions from the very beginning, see [11] for further insight. Another possible way to obtain (2.70) is to consider the internal energy to be a function of the entropy and the density with

$$\frac{\partial e}{\partial s} = T, \quad \text{and} \quad \frac{\partial e}{\partial \rho} = \frac{p}{\rho^2}. \tag{2.72}$$

If we now use (2.65) and exclude shock waves we obtain

$$\begin{aligned}
0 &= \frac{\partial}{\partial t}\mathcal{E} + \nabla_x \cdot (\mathbf{v}(\mathcal{E} + p)) = \frac{\partial}{\partial t}\left(\rho e + \rho\frac{\mathbf{v}^2}{2}\right) + \nabla_x \cdot \left[\left(\rho e + \rho\frac{\mathbf{v}^2}{2} + p\right)\mathbf{v}\right] \\
&= \rho T\left(\frac{\partial}{\partial t}s + \mathbf{v} \cdot \nabla_x s\right) + \frac{p}{\rho}\left(\frac{\partial}{\partial t}\rho + \mathbf{v} \cdot \nabla_x \rho\right) + \frac{\partial}{\partial t}\left(\rho\frac{\mathbf{v}^2}{2}\right) + \nabla_x \cdot \left[\left(\rho\frac{\mathbf{v}^2}{2} + p\right)\mathbf{v}\right] \\
&= \rho T\left(\frac{\partial}{\partial t}s + \mathbf{v} \cdot \nabla_x s\right) + sT\underbrace{\left(\frac{\partial}{\partial t}\rho + \nabla_x \cdot (\rho\mathbf{v})\right)}_{\overset{(2.63)}{=}0} - p\nabla_x \cdot \mathbf{v} \\
&\quad + \frac{\partial}{\partial t}\left(\rho\frac{\mathbf{v}^2}{2}\right) + \nabla_x \cdot \left[\left(\rho\frac{\mathbf{v}^2}{2} + p\right)\mathbf{v}\right] \\
&= T\left(\frac{\partial}{\partial t}(\rho s) + \nabla_x \cdot (\rho s\mathbf{v})\right)
\end{aligned}$$

In the (special) situation of the adiabatic Euler equations we can use minus the physical entropy $-s$ as mathematical entropy for the system. Since s is concave, see Section 1.2, the mathematical entropy is convex and minus the inequality (2.71) is the (mathematical) entropy inequality. Thus in the present case we have that shocks which are satisfying (2.71) also satisfy the Lax condition and vice versa, see also [85]. A detailed calculation showing this equivalence in the isothermal case can be found in Section 3.1.

In the case that the singular surface is assumed to support tension we have to consider $\mathbf{t}_{\mathcal{S}}^{i\alpha}$. Further we assume the surface entropy to depend on the temperature alone and hence obtain[21]

$$\begin{aligned} [\![\dot{m}]\!] &= 0, \\ \dot{m}\,[\![\mathbf{v}_i]\!] + [\![p]\!]\,\boldsymbol{\nu}_i &= \nabla_\alpha \mathbf{t}_{\mathcal{S}}^{i\alpha} \overset{(2.46)}{=} 2\sigma(T_{\mathcal{S}})K_M,\ i \in \{1,2,3\}, \\ \dot{m}\left[\!\!\left[e + \frac{p}{\rho} + \frac{1}{2}\left(\mathbf{v} - \mathbf{w}\right)^2\right]\!\!\right] &= 0 \\ \dot{m}\,[\![s]\!] &= \zeta_{\mathcal{S}} \geq 0. \end{aligned}$$

Note that the jump condition for the energy was again reformulated using the second equation. If the assumption of a time independent metric is dropped for example, then the additional term $\mathbf{t}_{\mathcal{S}}^{i\alpha}\nabla_\alpha \mathbf{w}_i$ occurs in the energy jump condition.

We now want to focus on the one dimensional case and exemplary apply some of the results of the previous Section 2.3 concerning the Riemann problem (2.60). For a very detailed discussion of the one dimensional Riemann problem for the adiabatic Euler equations, with a special emphasis on the thermodynamic properties and how they influence the solution structure, we highly recommend the work by Menikoff and Plohr [60].

Using the conservative variables $\mathbf{u} = (u_1, u_2, u_3) = (\rho, \rho \mathrm{v}, \mathcal{E})$ the flux function for the Euler system reads

$$\mathbf{F}(\mathbf{u}) = \begin{pmatrix} \rho \mathrm{v} \\ \rho \mathrm{v}^2 + p \\ \mathrm{v}(\mathcal{E} + p) \end{pmatrix} = \begin{pmatrix} u_2 \\ \dfrac{u_2^2}{u_1} + p \\ \dfrac{u_2}{u_1}(u_3 + p) \end{pmatrix}. \tag{2.73}$$

---

[21] In this case we have $\sigma \equiv f_{\mathcal{S}} = -T_{\mathcal{S}} s_{\mathcal{S}}$

Then the Jacobian is given by

$$\mathbf{A}(\mathbf{u}) = \begin{pmatrix} 0 & 1 & 0 \\ -\left(\frac{u_2}{u_1}\right)^2 + \frac{\partial p}{\partial u_1} & 2\frac{u_2}{u_1} + \frac{\partial p}{\partial u_2} & \frac{\partial p}{\partial u_3} \\ -\frac{u_2}{u_1^2}(u_3 + p) + \frac{u_2}{u_1}\frac{\partial p}{\partial u_1} & \frac{u_3 + p}{u_1} + \frac{u_2}{u_1}\frac{\partial p}{\partial u_2} & \frac{u_2}{u_1}\left(1 + \frac{\partial p}{\partial u_3}\right) \end{pmatrix}. \tag{2.74}$$

At this point we want to outline that the so called *homogeneity property* needed for the *Flux Vector Splitting* (cf. [78]) crucially depends on the chosen *EOS*. The homogeneity property is given by $\mathbf{A}(\mathbf{u})\mathbf{u} = \mathbf{F}(\mathbf{u})$. To investigate this we calculate $\mathbf{A}(\mathbf{u})\mathbf{u}$

$$\mathbf{A}(\mathbf{u})\mathbf{u} = \begin{pmatrix} u_2 \\ \frac{u_2^2}{u_1} + u_1\frac{\partial p}{\partial u_1} + u_2\frac{\partial p}{\partial u_2} + u_3\frac{\partial p}{\partial u_3} \\ \frac{u_2}{u_1}\left(u_3 + u_1\frac{\partial p}{\partial u_1} + u_2\frac{\partial p}{\partial u_2} + u_3\frac{\partial p}{\partial u_3}\right) \end{pmatrix}.$$

This expression is only equal to $\mathbf{F}(\mathbf{u})$ if

$$p \overset{!}{=} u_1\frac{\partial p}{\partial u_1} + u_2\frac{\partial p}{\partial u_2} + u_3\frac{\partial p}{\partial u_3} = \rho\frac{\partial p}{\partial \rho} + e\frac{\partial p}{\partial e}.$$

This means that p has to be a homogeneous function of degree one.
For the following calculations we assume that the pressure is given by an EOS of the form $p = p(\rho, e)$ [22]. Now we have using (2.27)

$$e(\mathbf{u}) = \frac{u_3}{u_1} - \frac{1}{2}\left(\frac{u_2}{u_1}\right)^2 \quad \text{with} \quad \mathrm{d}e = -\left(\frac{u_3}{u_1^2} - \frac{u_2^2}{u_1^3}\right)\mathrm{d}u_1 - \frac{u_2}{u_1^2}\mathrm{d}u_2 + \frac{1}{u_1}\mathrm{d}u_3. \tag{2.75}$$

Hence we obtain for the pressure $p(\mathbf{u})$

$$\mathrm{d}p = \left(\frac{\partial p}{\partial \rho} + \frac{\partial p}{\partial e}\frac{\partial e}{\partial u_1}\right)\mathrm{d}u_1 + \frac{\partial p}{\partial e}\frac{\partial e}{\partial u_2}\mathrm{d}u_2 + \frac{\partial p}{\partial e}\frac{\partial e}{\partial u_3}\mathrm{d}u_3. \tag{2.76}$$

---

[22] More precisely we should distinguish between the value of the pressure p and functions $\tilde{p}(\rho, e)$ and $\hat{p}(\mathbf{u})$ used to calculate it, i.e. $p = \tilde{p}(\rho, e) = \hat{p}(\mathbf{u})$. As mentioned earlier we do not make this distinction.

From (2.76) we obtain the useful relation

$$0 = \frac{\partial p}{\partial u_2} + \frac{\partial p}{\partial u_3}\frac{u_2}{u_1}.$$

The eigenvalues of (2.74) are given by

$$\lambda_{1/3}(\mathbf{u}) = \frac{u_2}{u_1} \pm \sqrt{\frac{\partial p}{\partial u_1} + \left(p + \frac{u_3}{u_1} - \left(\frac{u_2}{u_1}\right)^2\right)\frac{\partial p}{\partial u_3}}, \quad \lambda_2(\mathbf{u}) = \frac{u_2}{u_1} \tag{2.77}$$

To rewrite the eigenvalues, especially the radicand, we use (2.75) and (2.76) to obtain

$$\frac{\partial p}{\partial u_1} + \left(p + \frac{u_3}{u_1} - \left(\frac{u_2}{u_1}\right)^2\right)\frac{\partial p}{\partial u_3} = \frac{\partial p}{\partial \rho} + \frac{p}{\rho^2}\frac{\partial p}{\partial e}.$$

Using Lemma 1.3.7 (ii) one verifies that this is the square of the sound speed a. Hence we can rewrite the eigenvalues as

$$\lambda_1 = \mathrm{v} - \sqrt{a^2}, \quad \lambda_2 = \mathrm{v} \quad \text{and} \quad \lambda_3 = \mathrm{v} + \sqrt{a^2}.$$

These eigenvalues are real and distinct for suited EOS, cf. Section 1.3. The corresponding eigenvectors are

$$\mathbf{r}_1(\mathbf{u}) = \begin{pmatrix} 1 \\ \dfrac{u_2}{u_1} - a \\ \dfrac{p + u_3 - u_2 a}{u_1} \end{pmatrix}, \quad \mathbf{r}_2(\mathbf{u}) = \begin{pmatrix} 1 \\ \dfrac{u_2}{u_1} \\ -\dfrac{\partial_{u_1} p}{\partial_{u_3} p} + \left(\dfrac{u_2}{u_1}\right)^2 \end{pmatrix} \quad \text{and}$$

$$\mathbf{r}_3(\mathbf{u}) = \begin{pmatrix} 1 \\ \dfrac{u_2}{u_1} + a \\ \dfrac{p + u_3 + u_2 a}{u_1} \end{pmatrix}. \tag{2.78}$$

To find the Riemann invariants and further test whether the fields are genuine nonlinear or linearly degenerated we choose other (more convenient) variables. However, one could also use the conservative variables but the calculations would be more tedious. There are two choices which seem to be useful. The first choice we want to discuss is the case of the primitive variables (ρ, v, p). The choice of the density and the velocity is obviously due to the equations for mass and momentum. The pressure is convenient since it often occurs as independent thermodynamic variable. The Euler system can be reformulated by simply differentiating the equations, i.e.

$$\begin{aligned} \partial_t \rho + \mathrm{v}\partial_x \rho + \rho \partial_x \mathrm{v} &= 0, \\ \partial_t \mathrm{v} + \mathrm{v}\partial_x \mathrm{v} + \frac{1}{\rho}\partial_x p &= 0, \\ \partial_t p + \frac{1}{\partial_p e}\left(\frac{p}{\rho} - \rho\partial_\rho e\right)\partial_x \mathrm{v} + \mathrm{v}\partial_x p &= 0. \end{aligned} \tag{2.79}$$

Here we assumed that the internal energy is given by an EOS of the form $e = e(\rho, p)$. The Jacobian is then given by

$$\mathbf{A} = \begin{pmatrix} \mathrm{v} & \rho & 0 \\ 0 & \mathrm{v} & \frac{1}{\rho} \\ 0 & \frac{1}{\partial_p e}\left(\frac{p}{\rho} - \rho\partial_\rho e\right) & \mathrm{v} \end{pmatrix}. \tag{2.80}$$

We determine the following three distinct eigenvalues

$$\lambda_1 = \mathrm{v} - \sqrt{\frac{1}{\partial_p e}\left(\frac{p}{\rho^2} - \partial_\rho e\right)}, \quad \lambda_2 = \mathrm{v} \quad \text{and} \quad \lambda_3 = \mathrm{v} + \sqrt{\frac{1}{\partial_p e}\left(\frac{p}{\rho^2} - \partial_\rho e\right)}. \tag{2.81}$$

Again we verify that the radicand is the square of the sound speed by using Lemma 1.3.7 (iii). The corresponding eigenvectors are

$$\mathbf{r}_1 = \begin{pmatrix} 1 \\ -\frac{a}{\rho} \\ a^2 \end{pmatrix}, \quad \mathbf{r}_2 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \text{and} \quad \mathbf{r}_3 = \begin{pmatrix} 1 \\ \frac{a}{\rho} \\ a^2 \end{pmatrix}. \tag{2.82}$$

Now we can immediately verify that the second characteristic field is linearly degenerated, i.e.

$$\nabla_u \lambda_2 \cdot \mathbf{r}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = 0.$$

Thus the second wave is a contact discontinuity. Considering equation (2.55)$_2$ together with $\mathbf{r}_2$ we obtain that the Riemann invariants across the contact discontinuity are given by the pressure and the velocity. More precisely, the pressure and the velocity are continuous across the contact discontinuity, in particular the discontinuity also moves at the velocity $S = \mathrm{v}$. This implies for the mass flux $\dot{m} = \rho(\mathrm{v} - S) = 0$ and thus the jump conditions

$$\begin{aligned} [\![\dot{m}]\!] &= 0, \\ \dot{m}\underbrace{[\![\mathrm{v}]\!]}_{=0} + \underbrace{[\![p]\!]}_{=0} &= 0, \\ \dot{m}\left[\!\!\left[e + \frac{p}{\rho} + \frac{1}{2}(\mathrm{v} - S)^2 \right]\!\!\right] &= 0. \end{aligned}$$

hold as expected.

For further insight it is adequate to consider the entropy instead of the pressure, i.e. the primitive variables (ρ, v, s). This choice is quite favorable especially from a thermodynamic point of view, since we have the basic thermodynamic variables density (volume) and entropy as independent quantities. For smooth solutions the entropy is balanced by equation (2.70) and hence the entropy is conserved for the rarefaction wave. In particular the entropy is a Riemann invariant for the rarefaction wave as we shall see in a moment. Again the Euler system can be easily reformulated by simply differentiating the equations, i.e.

$$\begin{aligned} \partial_t \rho + \mathrm{v}\partial_x \rho + \rho \partial_x \mathrm{v} &= 0, \\ \partial_t \mathrm{v} + \mathrm{v}\partial_x \mathrm{v} + \frac{1}{\rho}\partial_x p &= 0, \\ \partial_t s + \mathrm{v}\partial_x s &= 0. \end{aligned} \tag{2.83}$$

Here we assumed that the internal energy is given in its fundamental form $e = e(\rho, s)$. The Jacobian is then given by

$$\mathbf{A} = \begin{pmatrix} \mathrm{v} & \rho & 0 \\ \frac{a^2}{\rho} & \mathrm{v} & \frac{\partial_s p}{\rho} \\ 0 & 0 & \mathrm{v} \end{pmatrix}. \tag{2.84}$$

We determine the following three distinct eigenvalues

$$\lambda_1 = \mathrm{v} - a, \quad \lambda_2 = \mathrm{v} \quad \text{and} \quad \lambda_3 = \mathrm{v} + a. \tag{2.85}$$

Due to the special choice of the variables we immediately obtain the sound speed a in our calculations. The corresponding eigenvectors are

$$\mathbf{r}_1 = \begin{pmatrix} 1 \\ -\dfrac{a}{\rho} \\ 0 \end{pmatrix}, \quad \mathbf{r}_2 = \begin{pmatrix} 1 \\ 0 \\ \dfrac{a^2}{\partial_s p} \end{pmatrix} \quad \text{and} \quad \mathbf{r}_3 = \begin{pmatrix} 1 \\ \dfrac{a}{\rho} \\ 0 \end{pmatrix}. \tag{2.86}$$

Again we can verify that the second characteristic field is linearly degenerated. That the pressure is constant in this case can now be obtained from the jump conditions, i.e. (2.67) together with $[\![\mathrm{v}]\!] = 0$. Now we verify that the first and third characteristic fields are genuine nonlinear. We yield

$$\nabla_u \lambda_{1/3} \cdot \mathbf{r}_{1/3} = \begin{pmatrix} \pm\dfrac{\partial a}{\partial \rho} \\ 1 \\ \pm\dfrac{\partial a}{\partial s} \end{pmatrix} \cdot \begin{pmatrix} 1 \\ \pm\dfrac{a}{\rho} \\ 0 \end{pmatrix} = \pm\left(\frac{\partial a}{\partial \rho} + \frac{a}{\rho}\right) = \pm\frac{1}{\rho}\frac{\partial(\rho a)}{\partial \rho} = \pm\frac{a}{\rho}\mathcal{G}. \tag{2.87}$$

For the last equation we used the chain rule and the results of Section 1.3 to obtain the fundamental derivative $\mathcal{G}$. It is a fundamental observation in [60] that whether the considered fields are genuine nonlinear or not is determined by a dimensionless quantity which is directly linked to the considered material. Here we will assume $\mathcal{G} > 0$ and thus the first and the third characteristic field are genuine nonlinear. A further observation was that the complete dynamics of the Riemann problem can be described using the dimensionless quantities defined in Definition 1.3.3. For example $\gamma \geq 0$ is needed for thermodynamic stability and for $\gamma > 0$ the Euler system is strictly hyperbolic. A complete discussion of all the different cases and their implications is beyond our scope and we again refer to [60]. Just note the difference between $\mathcal{G} < 0$ and $\mathcal{G} > 0$. In the latter (our) case the dynamics are as expected, i.e. the specific volume increases as the pressure decreases. Thus a rarefaction wave really rarefies a fluid. However, in the case $\mathcal{G} < 0$ the fluid is compressed by a "rarefaction wave". For this case we also exemplary refer to [67].

Now that we know that the first and third waves are genuine nonlinear we can discuss them in detail. In the case of a shock wave with speed S the Rankine-Hugoniot conditions (2.59) hold. For the rarefaction wave we immediately see that the entropy is a Riemann invariant. Further we obtain using (2.55)$_2$

$$\frac{\mathrm{d}\rho}{\mathrm{d}\xi} = \left(\pm\frac{a}{\rho}\mathcal{G}\right)^{-1} \quad \text{and} \quad \frac{\mathrm{d}\mathrm{v}}{\mathrm{d}\xi} = \left(\pm\frac{a}{\rho}\mathcal{G}\right)^{-1}\left(\pm\frac{a}{\rho}\right).$$

This gives together an equation for the second Riemann invariant $\mathcal{R}_\pm$, i.e.

$$\frac{\mathrm{d}\mathrm{v}}{\mathrm{d}\rho} = \pm\frac{a}{\rho} \quad \Leftrightarrow \quad \mathcal{R}_\pm = \mathrm{v} \pm \int_\rho \frac{a}{\sigma}\,\mathrm{d}\sigma. \tag{2.88}$$

Note that the second independent variable is given by the entropy and thus the integration is performed along an isentrope.

The Riemann problem may now be solved by connecting the initial states $\mathbf{u}_L$ and $\mathbf{u}_R$ using the obtained relations for the waves. The solution structure is depicted in Figure 2.6. The key idea is to construct curves in the velocity - pressure plane that reach every state that can be connected to the initial state $\mathbf{u}_L$ or $\mathbf{u}_R$ by a shock or rarefaction wave. Since the pressure and the velocity are constant across a contact discontinuity a solution is given by the intersection of such curves, see Figure 2.7. For a rarefaction wave we use the Riemann invariant given in (2.88) but now such that we use the pressure instead of the density for the integration. We obtain for a left and a right rarefaction wave

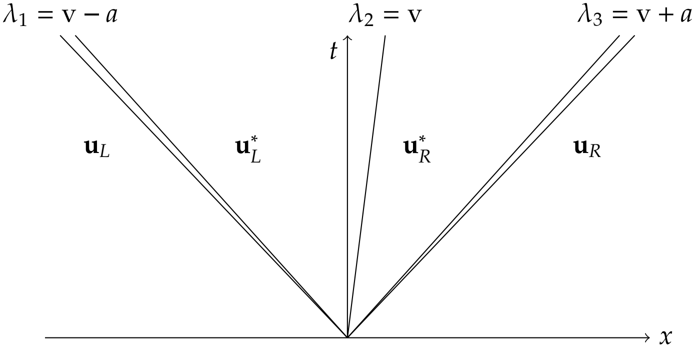

Figure 2.6: The solution structure of the Riemann problem.

$$\mathrm{v}_L^* = \mathrm{v}_L - \int_{p_L}^{p_L^*} \frac{1}{a\rho}\,\mathrm{d}p \quad \text{and} \quad \mathrm{v}_R^* = \mathrm{v}_R + \int_{p_R}^{p_R^*} \frac{1}{a\rho}\,\mathrm{d}p. \tag{2.89}$$

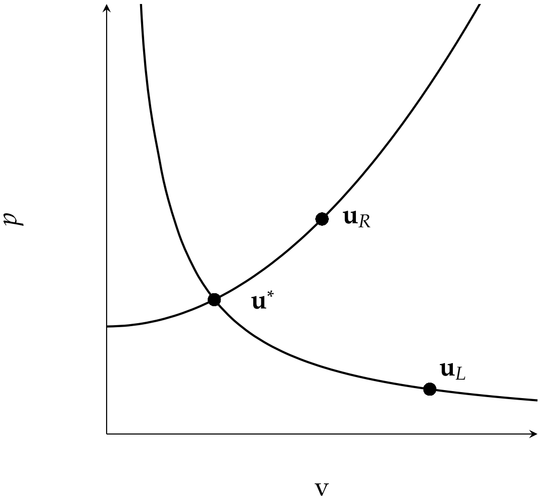

Figure 2.7: Intersecting wave curves for a Riemann problem.

For a shock wave we manipulate the Rankine-Hugoniot conditions (2.59) to obtain for a left and a right shock

$$\mathrm{v}_L^* = \mathrm{v}_L - \sqrt{\frac{[\![p]\!]\,[\![\rho]\!]}{\rho_L \rho_L^*}} \quad \text{and} \quad \mathrm{v}_R^* = \mathrm{v}_R + \sqrt{\frac{[\![p]\!]\,[\![\rho]\!]}{\rho_R \rho_R^*}}. \tag{2.90}$$

Additionally we use the jump condition for the energy and an EOS of the form $e(p, \rho)$

$$0 = [\![e(p,\rho)]\!] + \frac{1}{2}(p_R + p_L)\left[\!\!\left[\frac{1}{\rho}\right]\!\!\right]. \tag{2.91}$$

to eliminate the internal energy and obtain the density as a function of the pressure alone.
Finally, due to the conditions for a contact wave $p_R^* - p_L^* = [\![p]\!] = 0$ and $\mathrm{v}_R^* - \mathrm{v}_L^* = [\![\mathrm{v}]\!] = 0$ we can collapse them into a single equation for the

unknown pressure p^*, i.e.

$$f(p^*, \mathbf{u}_L, \mathbf{u}_R) = f_R(p^*, \mathbf{u}_R) + f_L(p^*, \mathbf{u}_L) + \mathrm{v}_R - \mathrm{v}_L = 0, \tag{2.92}$$

$$f_K(p, \mathbf{u}_K) = \begin{cases} \sqrt{\dfrac{[\![p]\!]\,[\![\rho]\!]}{\rho(p)\rho_K}},\ p > p_K \text{ (Shock)} \\ \displaystyle\int_{p_K}^{p} \frac{1}{a(\zeta)\rho(\zeta)}\,\mathrm{d}\zeta,\ p \le p_K \text{ (Rarefaction)} \end{cases}, \quad K \in \{L, R\}.$$

Throughout these calculations we assumed an EOS that links the thermodynamic variables in a suited way, see Section 1.3. Thus we reduced the problem of solving the Riemann problem to finding a root of a nonlinear one dimensional equation. We want to close this brief discussion with the remark that this root does not necessarily has to exist, see the afore mentioned literature. A similar discussion for the isothermal case is given in Section 3.1 and for the isentropic case we omit such a presentation.

2.4.2 Isothermal Euler Equations

Often the isothermal Euler equations are discussed as if they are a submodel of the Euler equations obtained above. This might be justified from a numerical point of view, but it is surely not from a physical point of view. There are several reasons for this remark. First we assumed $\mathbf{q} \equiv 0$ to obtain the Euler equations, but an isothermal process *needs* heat exchange to keep the temperature constant. That this can be seen mathematically by analyzing the energy equations (2.29) and (2.65) is the second point. Further we only assume $\rho_{\mathcal{S}} \equiv 0$. Thus the corresponding conditions for singular surfaces are obtained fairly easy.

The isothermal Euler equations are given by

$$\frac{\partial}{\partial t}\rho + \nabla_x \cdot (\rho \mathbf{v}) = 0, \tag{2.93}$$

$$\frac{\partial}{\partial t}(\rho \mathbf{v}_i) + \nabla_x \cdot \left(\rho \mathbf{v}_i \mathbf{v} + p\mathbf{e}^{(\mathbf{i})}\right) = 0,\ i \in \{1, 2, 3\}, \tag{2.94}$$

The total energy balance (2.29) determines the heat flux, i.e.

$$\frac{\partial}{\partial t}\mathcal{E} + \nabla_x \cdot (\mathbf{v}\,(\mathcal{E} + p) + \mathbf{q}) = 0$$

$$\nabla_x \cdot \mathbf{q} = -\left(\frac{\partial}{\partial t}\left(\rho e + \rho\frac{\mathbf{v}^2}{2}\right) + \nabla_x \cdot \left[\left(\rho e + \rho\frac{\mathbf{v}^2}{2} + p\right)\mathbf{v}\right]\right). \tag{2.95}$$

If we combine the entropy balance (2.35) with (2.95) we yield for $T = const.$

$$\begin{aligned}
0 \le \zeta &= \frac{\partial}{\partial t}(\rho s) + \nabla_x \cdot \left(\rho s \mathbf{v} + \frac{\mathbf{q}}{T}\right) \\
&= \frac{\partial}{\partial t}(\rho s) + \nabla_x \cdot (\rho s \mathbf{v}) - \frac{1}{T}\left(\frac{\partial}{\partial t}\left(\rho e + \rho\frac{\mathbf{v}^2}{2}\right) + \nabla_x \cdot \left[\left(\rho e + \rho\frac{\mathbf{v}^2}{2} + p\right)\mathbf{v}\right]\right) \\
&= -\frac{1}{T}\left(\frac{\partial}{\partial t}\left(\rho(e - Ts) + \rho\frac{\mathbf{v}^2}{2}\right) + \nabla_x \cdot \left[\left(\rho\left(e - Ts + \frac{p}{\rho}\right) + \rho\frac{\mathbf{v}^2}{2}\right)\mathbf{v}\right]\right).
\end{aligned}$$

This is equivalent to

$$0 \ge -T\zeta = \frac{\partial}{\partial t}\left(\rho(e - Ts) + \rho\frac{\mathbf{v}^2}{2}\right) + \nabla_x \cdot \left[\left(\rho\left(e - Ts + \frac{p}{\rho}\right) + \rho\frac{\mathbf{v}^2}{2}\right)\mathbf{v}\right]. \tag{2.96}$$

Note that $e - Ts$ is the specific free energy f and $f + p/\rho$ the Gibbs energy of the bulk phase. This indeed is the stability condition for a thermodynamic system with uniform and constant temperature. According to [64] (§ 1.4.2, pp. 23) it states that: "*The sum of the free energy and kinetic energy tends to a minimum under the constraints of constant mass and constant and uniform temperature.* [23]

The corresponding jump conditions across discontinuities are given by (2.66) and

$$\dot{m}\,[\![\mathbf{v}_i]\!] + [\![p]\!]\,\boldsymbol{\nu}_i = S^{\alpha\beta} b_{\alpha\beta},\ i \in \{1, 2, 3\}, \tag{2.97}$$

Where $S^{\alpha\beta}$ is given by (2.46) with $\rho_{\mathcal{S}} \equiv 0$. The entropy inequality for the singular surface is obtained from (2.44) and thus given by

$$-\dot{m}\left[\!\!\left[g + \underbrace{\frac{1}{2}(\mathbf{v} - \mathbf{w})^2}_{=e_{kin}} \right]\!\!\right] = T\zeta_{\mathcal{S}} \ge 0. \tag{2.98}$$

Note that this agrees with the flux term in (2.96). That this (mathematical) entropy inequality is equivalent to the Lax criterion is shown in Section 3.1.

---

[23] This is analogue to the situation in equilibrium. Neglect for moment the kinetic energy and further consider the volume to be constant. Then one obtains $0 \ge \partial_t(\rho f) + \nabla_x \cdot (\rho f \mathbf{v}) = \mathrm{d}F/\mathrm{d}t$. Hence in equilibrium the free energy of a system is minimized. This result can be found in the literature, cf. [52, 70].

2.4.3 Isentropic Euler Equations

For the isentropic Euler equations we have no contributions on the right hand side of equation (2.1) and (2.5), respectively. Thus the entropy balances reduce to

$$\frac{\partial}{\partial t}(\rho s) + \nabla_x \cdot (\rho s \mathbf{v}) = 0, \tag{2.99}$$

$$\frac{\partial}{\partial t} s_{\mathcal{S}} + s_{\mathcal{S}} \left(\nabla_\alpha w_\tau^\alpha - 2K_M w_\nu\right) + [\![\dot{m} s]\!] = 0. \tag{2.100}$$

From Section 1.1 we know that the internal energy and the entropy are related by the complete differential

$$\mathrm{d}e = \frac{1}{T}\mathrm{d}s + \frac{p}{\rho^2}\mathrm{d}\rho$$

and thus we have for an isentropic process

$$\mathrm{d}e = \frac{p}{\rho^2}\mathrm{d}\rho.$$

With this we obtain for the total energy balance as before (with $\mathbf{q} \equiv 0$)

$$\begin{aligned}
0 &= \frac{\partial}{\partial t}\mathcal{E} + \nabla_x \cdot ((\mathcal{E} + p)\,\mathbf{v}) = \frac{\partial}{\partial t}\left(\rho e + \rho\frac{\mathbf{v}^2}{2}\right) + \nabla_x \cdot \left[\left(\rho e + \rho\frac{\mathbf{v}^2}{2} + p\right)\mathbf{v}\right] \\
&= \frac{\partial}{\partial t}(\rho e) + \nabla_x \cdot (\rho e \mathbf{v}) + \frac{\partial}{\partial t}\left(\rho\frac{\mathbf{v}^2}{2}\right) + \nabla_x \cdot \left[\left(\rho\frac{\mathbf{v}^2}{2} + p\right)\mathbf{v}\right] \\
&= \rho\left(\frac{\partial e}{\partial \rho}\right)_s \left(\frac{\partial}{\partial t}\rho + \mathbf{v} \cdot \nabla_x \rho\right) + \frac{\partial}{\partial t}\left(\rho\frac{\mathbf{v}^2}{2}\right) + \nabla_x \cdot \left[\left(\rho\frac{\mathbf{v}^2}{2} + p\right)\mathbf{v}\right] \\
&= -\rho^2\left(\frac{\partial e}{\partial \rho}\right)_s \nabla_x \cdot \mathbf{v} + \frac{\partial}{\partial t}\left(\rho\frac{\mathbf{v}^2}{2}\right) + \nabla_x \cdot \left(\frac{1}{2}\rho\mathbf{v}^2\mathbf{v} + p\mathbf{v}\right) \\
&= \frac{\partial}{\partial t}\left(\rho\frac{\mathbf{v}^2}{2}\right) + \nabla_x \cdot \left(\frac{1}{2}\rho\mathbf{v}^2\mathbf{v} + p\mathbf{v}\right) - p\nabla_x \cdot \mathbf{v}.
\end{aligned}$$

Which is the balance for the kinetic energy (2.25) and thus it is redundant. Therefore the isentropic Euler equations are given by (2.63) and (2.64), i.e.

$$\begin{gathered}
\frac{\partial}{\partial t}\rho + \nabla_x \cdot (\rho \mathbf{v}) = 0, \\
\frac{\partial}{\partial t}(\rho \mathbf{v}^i) + \nabla_x \cdot \left(\rho \mathbf{v}^i \mathbf{v} + p\mathbf{e}^{(\mathbf{i})}\right) = 0,\ i \in \{1, 2, 3\}.
\end{gathered}$$

The analogy to the adiabatic Euler equations is no incident. In fact away from shocks the entropy is conserved for the adiabatic Euler equations as we have seen before. If we thus further make the same assumptions for the jump conditions as for the adiabatic Euler equations we obtain the following

$$\begin{aligned} [\![\dot{m}]\!] &= 0, \\ \dot{m}\,[\![\mathbf{v}_i]\!] + [\![p]\!]\,\boldsymbol{\nu}_i &= 0, \; i \in \{1,2,3\}, \\ \dot{m}\,[\![s]\!] &= 0. \end{aligned}$$

The difference between the isothermal and the isentropic case becomes apparent in the EOS, the entropy inequalities and the total energy balance.

Part II

Isothermal Case

Introduction

In the second part of this work we now want to discuss *isothermal two-phase flows*, in particular isothermal liquid-vapor flows. Such compressible liquid-vapor flows have a wide range of applications. Two-phase flow models are used to describe such processes, e.g. the formation of clouds, cavitation near moving objects in liquids such as ship propellers or certain phenomena in biology. Main difficulties in the modeling result from the phase interactions, especially from mass and energy transfer due to condensation or evaporation processes.

Several two-phase flow models are available in the literature. They are mainly distinguished in sharp and diffusive interface models. For a detailed discussion of these models we refer to Zein [87] and concerning sharp interface models we exemplary refer to Bedeaux et al. [8]. In our work we study compressible two-phase flows with phase transitions across a sharp interface. Phase transitions are modeled using a kinetic relation. This concept was introduced by Abeyaratne and Knowles [1] for solid-solid phase transitions. This kinetic relation controls the mass transfer across the interface between the two adjacent phases. For a more general context of kinetic relations see LeFloch [55]. As mentioned before an interesting survey on the Riemann problem for a large class of thermodynamic consistent constitutive models in the setting of Euler equations models can be found in Menikoff and Plohr [60]. In this work the considerations are restricted to a simple kinetic relation that results from the assumption of local equilibrium at the interface.

In a recent work by Hantke et al. [37] Riemann problems relying on the isothermal Euler equations with a non-monotone pressure-density function are considered. This function is composed of three parts: the equations of state for the two single phases and an arbitrary relation for the intermediate state. The two phases are distinguished using the Maxwell construction, also known as the Equal-Area-Rule. The mass transfer is modeled via a kinetic relation, derived in [23], based on classical Hertz-Knudsen theory, see [10]. The authors discussed Riemann problems for various different cases of initial data and showed existence and uniqueness. Furthermore Hantke et al. also covered the cases of cavitation and nucleation. The constructed Riemann solutions are selfsimilar. They consist of constant states, separated by classical rarefaction or shock waves and phase boundaries. Nevertheless, the basic assumptions are very restrictive. Existence and uniqueness results are proven for liquid water and its vapor, modeled by linear equations of state. Also Müller and Voss [67], [81] considered the isothermal Euler system. In contrast to the above mentioned work they modeled the fluid using the van der Waals equation of state. Instead of a kinetic relation the Liu entropy condition is used to achieve uniqueness. As a consequence Müller and Voss need non-classical composite waves to construct solutions. A further reference for vapor - liquid phase transitions in the context of conservation laws is the detailed review by Fan and Slemrod [30]. They also treat the isothermal case using the method of vanishing viscosity applied to the Lagrange formulation of the conservation laws. Additional literature in this context is given by Merkle [61], Merkle and Rohde [62].

Considering the work of Hantke et al. [37] several questions follow. In this part we want to consider the following two questions.
First, in Chapter 3 we generalize the results obtained in [37] to arbitrary equations of state. Therefore we focus on physically reasonable EOS and refer to the results obtained in the previous part, especially Chapter 1. Chapter 3 is a slightly extended version of the following work[24]

[41] M. Hantke and F. Thein. A general existence result for isothermal two-phase flows with phase transition. *ArXiv e-prints*, Mar. 2017

The second question that arises is the numerical treatment. Due to the novel approach there are only few methods available to cover all the dynamics discussed in the analytical treatment. Hence in Chapter 4 we present a numerical approach for solving the Riemann problem presented in Chapter 3. The presented numerical method is capable to solve the two phase problems including nucleation and cavitation. Parts of Chapter 4 have been published in

[38] M. Hantke and F. Thein. Numerical solutions to the Riemann problem for compressible isothermal Euler equations for two phase flows with and without phase transition. In *Hyperbolic problems: theory, numerics, applications*, volume 8 of *AIMS Ser. Appl. Math.*, pages 651–658. AIMS, 2014

We want to note that in the present work we explain the method in more

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[24] Currently this work is submitted.

detail and also apply it to the results obtained in Chapter 3. In particular we are not restricted to the case of the two specific EOS chosen in [37].

3 Isothermal Case: Analytical Solution of the Riemann Problem

Introduction

The focus of the present chapter is on the distinguished generalization of the results of Hantke et al. [37] resp. Menikoff and Plohr [60].
We consider two-phase flows for any regular fluid. Both phases can be modeled by any thermodynamic reasonable equation of state. Further we construct exact Riemann solutions and prove existence and uniqueness results that advance achievements in the present literature.
The chapter is organized as follows. In Section 3.1 we summarize results for the balance equations in the bulk phases and the corresponding jump conditions across discontinuities. We will proceed along the ideas of the Sections 2.3 and 2.4. Further we will also summarize the thermodynamic framework needed throughout this chapter and discuss the Riemann problem in the isothermal case including the entropy inequality. Therefore we refer to the Sections 1.3 and 1.4. In Section 3.2 we prove existence and uniqueness of a solution at the interface under certain appropriate assumptions. The following Section 3.3 contains a monotonicity argument needed to solve the two-phase Riemann problem, which is done subsequently. In Section 3.4 we present solutions to initial one-phase Riemann data leading to nucleation or cavitation, i.e. the creation of a new phase. We conclude this work with Section 3.5 where we give a detailed discussion of the assumptions made to state the previous results followed by some examples and the conclusion.

3.1 Isothermal Euler Equations

In this section we study inviscid, compressible and isothermal two phase flows.The two phases are either the liquid or the vapor phase of one substance. The phases are distinguished by the *mass density* ρ and further described by the *velocity* u. Sometimes it is convenient to use the *specific volume* $v = 1/\rho$ instead of the mass density. We will make the reader aware of such situations. The physical quantities depend on time $t \in \mathbb{R}_{\geq 0}$ and space $x \in \mathbb{R}$. In regular points of the bulk phases the fluid is described using the (one dimensional) isothermal Euler equations introduced in 2.4.2, i.e.

$$\partial_t \rho + \partial_x(\rho u) = 0, \tag{3.1}$$

$$\partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0. \tag{3.2}$$

Accordingly we have the following jump conditions across discontinuities

$$[\![\rho(u - W)]\!] = 0, \tag{3.3}$$

$$\rho(u - W)\,[\![u]\!] + [\![p]\!] = 0. \tag{3.4}$$

Furthermore every discontinuity satisfies the following entropy inequality

$$\rho(u - W)\left[\!\!\left[g + e^{kin}\right]\!\!\right] \leq 0. \tag{3.5}$$

The quantity W is the speed of the discontinuity and $Z = -\rho(u - W)$ the mass flux where we will distinguish between a classical shock wave and the phase boundary (non-classical shock)

$$Z = \begin{cases} Q, & \text{shock wave} \\ z, & \text{phase boundary} \end{cases} \quad \text{and} \quad W = \begin{cases} S, & \text{shock wave} \\ w, & \text{phase boundary} \end{cases}.$$

3.1.1 Definition and Requirements for the *EOS*

Concerning the thermodynamic requirements we refer to the first part of this work, in particular Chapter 1. Thus we will only give a brief summary of the results that are needed in the given context.

Usually one only works with the pressure law when dealing with the Euler equations. Nevertheless it was shown in 1.3 that the pressure law does not contain all the information about a fluid or more general a thermodynamic system. From a thermodynamic point of view a system in (local) equilibrium can be described relating the extensive quantities *energy* E, *volume* V

and *entropy* S, i.e. $E(V,S)$. In the following we will use the corresponding (intensive) densities and thus we use small letters (e.g.: e, v, s). Given this relation every other quantity can be derived using the first and second law of thermodynamics 1.1.2, 1.1.3 and the Maxwell relations (1.19) - (1.22). A discussion using the ideal gas EOS and the Tait EOS can also be found in [23]. From this point on we assume that we have an EOS for each phase with consistent thermodynamic properties. In view of Section 1.4 and (3.5) the thermodynamic potential we will consider here is the Gibbs energy (1.13). Its differential is given by (1.17), i.e.

$$\mathrm{d}g = -s\mathrm{d}T + v\mathrm{d}p.$$

Further the isothermal sound speed is given by (1.36)

$$a = \sqrt{-v^2\left(\frac{\partial p}{\partial v}\right)_T}.$$

Combining the previous two equations we obtain

$$\left(\frac{\partial g}{\partial p}\right)_T = v > 0, \quad \left(\frac{\partial^2 g}{\partial p^2}\right)_T = \left(\frac{\partial v}{\partial p}\right)_T = -\left(\frac{v}{a}\right)^2 < 0. \tag{3.6}$$

As noted earlier thermodynamic quantities may be expressed using different choices of independent variables. Thus the brackets with the subscript simply denote which quantity is held constant when calculating the derivative. In the isothermal case the Gibbs potential just depends on the pressure and hence we omit writing the brackets with subscript T. Here the volume v and the speed of sound a are strictly positive functions of the pressure p. Furthermore the inequality for the second derivative is due to the requirement of thermodynamic stability for an isothermal system. In short this can be seen by considering the requirements for the full case. There, thermodynamic stability requires the energy to be a convex function, both in the entropy and the volume, see also 1.2. This implies that the Hessian of the energy is non negative. If we now assume the temperature to be constant, what remains is

$$0 \leq \frac{\mathrm{d}^2 e}{\mathrm{d}v^2} = -\frac{\mathrm{d}p}{\mathrm{d}v}. \tag{3.7}$$

In the following we use the subscripts $\{V, L\}$ when it is necessary to distinguish the vapor and the liquid phase. Since we are concerned with two phases we write g_L for the Gibbs energy of the liquid phase and g_V for the vapor phase, respectively. Further we require

$$\frac{\partial g_i}{\partial p_j} = 0, \ i \neq j, \ i, j \in \{V, L\}.$$

Since we only consider one substance the condition for two phases to be in equilibrium is according to (1.55)

$$g_L(p_L) = g_V(p_V). \tag{3.8}$$

Due to the monotonicity of $g_K, \ K \in \{V, L\}$ we have

$$g_L(p_L) = g_V(p_V) \quad \Leftrightarrow \quad p_L = p_V$$

and we write in this case

$$p_L = p_V =: p_0 \quad \text{and} \quad g_L(p_0) = g_V(p_0).$$

A crucial point when dealing with different phases is how to discriminate them and how to connect them thermodynamically consistent. Equations of state describing two phases (e.g. *van der Waals* EOS) have a so called spinodal region which is avoided by the Maxwell construction (or equal area rule) (1.60), see Section 1.4. We want to discriminate the phases using the specific volumes. Therefore we need an upper bound for the liquid volume v_m and a lower bound for the vapor volume $\tilde{v}$. This should still be consistent with the Maxwell construction. Therefore we may proceed as follows. We use the EOS for each phase and prescribe the minimum liquid pressure p_{min} (e.g. $p_{min} = 0$) and from this we obtain v_m. Further we know the saturation pressure p_0 for a given temperature T_0 from a calculation or from tables which are available for many substances, such as for water [84]. Now we connect our two EOS monotonically and then obtain the maximum vapor pressure $\tilde{p}$ according to Definition 1.4.1.
Finally, analogous to [60] we introduce dimensionless quantities which we will use later on. These quantities are given as in Definition 1.3.3. In particular we need the (isothermal) dimensionless speed of sound (1.29)

$$\gamma := -\frac{v}{p}\frac{\mathrm{d}p}{\mathrm{d}v}.$$

and the (isothermal) fundamental derivative (1.30)

$$\mathcal{G} := -\frac{1}{2} v \frac{\frac{\mathrm{d}^2 p}{\mathrm{d}v^2}}{\frac{\mathrm{d}p}{\mathrm{d}v}}.$$

We want to recall Remark 1.3.4 to emphasize the difference between the isothermal γ and the adiabatic γ_S, i.e.

$$\frac{\gamma}{\gamma_S} = \frac{c_V}{c_p}$$

and hence $\gamma \leq \gamma_S$ for thermodynamic stable systems. Further we have for γ, using (1.17) and (1.36)

$$\gamma = \frac{a^2}{pv}. \tag{3.9}$$

For the fundamental derivative one may also write

$$\mathcal{G} = \frac{1}{2} \frac{v^2}{p\gamma} \frac{\mathrm{d}^2 p}{\mathrm{d}v^2} = -\frac{v}{a} \frac{\mathrm{d}a}{\mathrm{d}v} + 1 \tag{3.10}$$

or when expressed in terms of the pressure

$$\mathcal{G} = \frac{a}{v} \frac{\mathrm{d}a}{\mathrm{d}p} + 1. \tag{3.11}$$

The *isotherms* in the $p - v$ plane are convex if $\mathcal{G} > 0$. This will be assumed from now on for both phases [1].

3.1.2 Riemann Problem

In the following we briefly discuss the solution of the Riemann problem for the isothermal Euler equations (3.1) and (3.2) for a single phase. In order to do so we will discuss the elementary wave types that can occur, which are

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[1] For examples of materials that have a convex or a nonconvex EOS we refer to the listing in Ben-Dor et al. [9].

shock or rarefaction waves. The Riemann problem is given by equations (3.1), (3.2), the EOS and the Riemann initial data

$$\rho(x,0) = \begin{cases} \rho_-, \, x < 0 \\ \rho_+, \, x > 0 \end{cases} \quad \text{and} \quad u(x,0) = \begin{cases} u_-, \, x < 0 \\ u_+, \, x > 0 \end{cases}. \tag{3.12}$$

We rewrite the system (3.1) and (3.2) in quasilinear form in terms of the primitive variables, i.e. the density ρ and the velocity u

$$\begin{pmatrix} \rho \\ u \end{pmatrix}_t + \begin{pmatrix} u & \rho \\ \frac{a^2}{\rho} & u \end{pmatrix} \begin{pmatrix} \rho \\ u \end{pmatrix}_x = 0. \tag{3.13}$$

The Jacobian matrix

$$\mathbf{A} = \begin{pmatrix} u & \rho \\ \frac{a^2}{\rho} & u \end{pmatrix} \tag{3.14}$$

has the following eigenvalues and corresponding eigenvectors

$$\lambda_1 = u - a, \quad \mathbf{r}_1 = \begin{pmatrix} \rho \\ -a \end{pmatrix}, \quad \lambda_2 = u + a, \quad \mathbf{r}_2 = \begin{pmatrix} \rho \\ a \end{pmatrix}. \tag{3.15}$$

Due to the requirement of thermodynamic stability (3.7) this system is hyperbolic. We have strict hyperbolicity for

$$\gamma > 0. \tag{3.16}$$

Furthermore one can immediately verify that the waves corresponding to the eigenvalues and eigenvectors are genuine nonlinear if and only if the fundamental derivative

$$\mathcal{G} = \frac{\rho}{a} \frac{\mathrm{d}a}{\mathrm{d}\rho} + 1.$$

does not vanish, i.e.

$$\nabla \lambda_{1/2} \cdot \mathbf{r}_{1/2} = \mp \frac{a}{\rho} \mathcal{G} \neq 0. \tag{3.17}$$

Here this is in fact the case, since we assumed $\mathcal{G} > 0$. For systems with genuine nonlinear waves the Lax condition is enough to pick the right solution, cf. [55] and also [60] for the full system. The Riemann invariants for this system are

$$\mathcal{R}_1 = u + \int \frac{a}{\rho} \, \mathrm{d}\rho \quad \text{and} \quad \mathcal{R}_2 = u - \int \frac{a}{\rho} \, \mathrm{d}\rho. \tag{3.18}$$

Entropy Inequality across a Shock Wave

In what follows we prove, that the Lax condition is equivalent to the entropy condition for an isothermal system. We consider two states

$$\begin{pmatrix}\rho_1\\ u_1\end{pmatrix} \quad \text{and} \quad \begin{pmatrix}\rho_2\\ u_2\end{pmatrix}$$

separated by a shock wave moving with speed S. Further we will also use the specific volume $v = 1/\rho$. Using the continuity of the mass flux and $Q = -\rho(u - S)$

$$u_2 - S = -\frac{Q}{\rho_2} = -v_2 Q, \quad u_1 - S = -\frac{Q}{\rho_1} = -v_1 Q \Rightarrow [\![u]\!] = -Q\,[\![v]\!]\,. \tag{3.19}$$

From the second jump condition (3.4) we obtain

$$Q = \frac{[\![p]\!]}{[\![u]\!]}$$

Combining this with (3.19) gives

$$Q^2 = -\frac{[\![p]\!]}{[\![v]\!]}. \tag{3.20}$$

Further we can also derive

$$[\![u]\!]^2 = -\,[\![p]\!]\,[\![v]\!]\,. \tag{3.21}$$

The entropy inequality is given by (3.5)

$$Q\left[\!\!\left[g + e^{kin}\right]\!\!\right] = -\rho(u - S)\left[\!\!\left[g + e^{kin}\right]\!\!\right] \geq 0.$$

Manipulating the bracket by using (3.19) results in

$$\left[\!\!\left[g + e^{kin}\right]\!\!\right] = \left[\!\!\left[g - \frac{1}{2}p(v_2 + v_1)\right]\!\!\right].$$

To discuss this expression we write it as function of p and calculate the first and second derivative

$$f(p) = g(p) - g(p_1) - \frac{1}{2}(p - p_1)(v(p) + v_1),$$

$$f'(p) = \frac{1}{2}\left\{v(p) - v_1 + (p - p_1)\left(\frac{v(p)}{a(p)}\right)^2\right\},$$

$$f''(p) = -(p - p_1)\frac{v(p)^3}{a(p)^4}\mathcal{G}.$$

We immediately see that

$$f(p_1) = 0, \; f'(p_1) = 0 \text{ and } f''(p_1) = 0$$

and hence, also using the derivatives, we can conclude

$$\llbracket g + e^{kin} \rrbracket \begin{cases} < 0, & p_2 > p_1 \\ = 0, & p_2 = p_1 \\ > 0, & p_2 < p_1 \end{cases}. \tag{3.22}$$

In order to derive the Lax condition we consider (3.20) and discuss the following function

$$f_Q(p) = -\frac{p - p_1}{v(p) - v(p_1)} \quad \text{with} \quad f_Q(p_2) = Q^2.$$

We yield for f_Q

$$f_Q'(p) = -\frac{(v(p) - v_1) + (p - p_1)\dfrac{v(p)^2}{a(p)^2}}{(v(p) - v_1)^2}.$$

The numerator is strictly monotone decreasing for every $p > p_1$ and thus

$$0 > (v(p) - v_1) + (p - p_1)\frac{v(p)^2}{a(p)^2}.$$

This, in turn, gives for $p = p_2$

$$0 = \llbracket p \rrbracket + Q^2 \llbracket v \rrbracket > \llbracket p \rrbracket + \llbracket v \rrbracket \frac{a(p_2)^2}{v(p_2)^2} \quad \Leftrightarrow \quad Q^2 < \frac{a(p_2)^2}{v(p_2)^2}.$$

Due to the monotonicity of g we further have

$$Q^2 > \lim_{p \to p_1} g(p) = -\lim_{p \to p_1} \frac{p - p_1}{v(p) - v_1} \overset{\text{l'Hospital}}{=} \lim_{p \to p_1} \frac{a(p)^2}{v(p)^2} = \frac{a(p_1)^2}{v(p_1)^2}.$$

All together we obtained

$$\frac{a(p_1)^2}{v(p_1)^2} < Q^2 < \frac{a(p_2)^2}{v(p_2)^2}. \tag{3.23}$$

Now obtaining the correct sign from the entropy inequality (3.5) and (3.22) applied to (3.19) with (3.23) gives the Lax condition for a left Shock ($Q > 0$) and a right shock ($Q < 0$), respectively. Therefore we have that in the isothermal case the Lax condition and the entropy inequality are equivalent.

Rarefaction Wave

For a rarefaction wave we use the Riemann invariants (3.18) and hence obtain for a left rarefaction wave (corresponding to λ_1)

$$u_2 - u_1 = -\int_{\rho_1}^{\rho_2} \frac{a}{\rho}\,\mathrm{d}\rho. \tag{3.24}$$

Furthermore the slope inside the rarefaction is given by

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{x}{t} = \lambda_1 = u - a \tag{3.25}$$

and hence we obtain that the solution inside the rarefaction fan is given by

$$u = \frac{x}{t} + a \quad \text{and} \quad F(\rho) = u - u_1 + \int_{\rho_1}^{\rho} \frac{a}{\sigma}\,\mathrm{d}\sigma = 0. \tag{3.26}$$

Here ρ is obtained as the root of $F(\rho)$. Similar we obtain the results for a right rarefaction

$$\begin{aligned} u_2 - u_1 &= \int_{\rho_1}^{\rho_2} \frac{a}{\rho}\,\mathrm{d}\rho, \quad \frac{\mathrm{d}x}{\mathrm{d}t} = \frac{x}{t} = \lambda_2 = u + a, \\ u &= \frac{x}{t} - a \quad \text{and} \quad F(\rho) = u_2 - u - \int_{\rho}^{\rho_2} \frac{a}{\sigma}\,\mathrm{d}\sigma = 0. \end{aligned} \tag{3.27}$$

Shock Wave

The relation across a shock wave is given by (3.21)

$$[\![u]\!]^2 = -[\![p]\!]\,[\![v]\!] = \frac{[\![p]\!]\,[\![\rho]\!]}{\rho_1\rho_2} \quad \Leftrightarrow \quad [\![u]\!] = -\sqrt{-[\![p]\!]\,[\![v]\!]} = -\sqrt{\frac{[\![p]\!]\,[\![\rho]\!]}{\rho_1\rho_2}}.$$

Solution of the Riemann Problem

If we now want to solve the Riemann problem for the isothermal Euler equations we just have to connect the three constant states separated by the waves using the equations obtained above. Therefore we assume the left and right state to be given and use that the velocity between the waves is constant. The solution is obtained as the root of the following function

$$f(\rho, W_L, W_R) = f_R(\rho, W_R) + f_L(\rho, W_L) + u_R - u_L = 0, \tag{3.28}$$

$$f_K(\rho, W_K) = \begin{cases} \sqrt{\dfrac{\llbracket p \rrbracket \llbracket \rho \rrbracket}{\rho \rho_K}}, \ \rho > \rho_K \text{ (Shock)} \\ \displaystyle\int_{\rho_K}^{\rho} \frac{a(\sigma)}{\sigma} \, \mathrm{d}\sigma, \ \rho \leq \rho_K \text{ (Rarefaction)} \end{cases}, \quad K \in \{L, R\}.$$

Due to $p'(\rho) > 0$ we could also state this problems in terms of the unknown pressure p, i.e.

$$f(p, W_L, W_R) = f_R(p, W_R) + f_L(p, W_L) + u_R - u_L = 0, \tag{3.29}$$

$$f_K(p, W_K) = \begin{cases} \sqrt{- \llbracket p \rrbracket \llbracket v \rrbracket}, \ p > p_K \text{ (Shock)} \\ \displaystyle\int_{p_K}^{p} \frac{v(\zeta)}{a(\zeta)} \, \mathrm{d}\zeta, \ p \leq p_K \text{ (Rarefaction)} \end{cases}, \quad K \in \{L, R\}.$$

In order to investigate $f(p, W_L, W_R)$ we need information about the asymptotic behavior

$$v(p) \overset{p\to\infty}{\longrightarrow} 0, \quad v(p) \overset{p\to 0}{\longrightarrow} \infty \quad \text{and further} \quad \frac{\mathrm{d}v(p)}{\mathrm{d}p} \overset{(3.6)_2}{=} -\frac{v(p)^2}{a(p)^2} < 0.$$

We obtain for $f_K(p, W_K)$ in the case of a shock wave

$$\frac{\mathrm{d}}{\mathrm{d}p} f_K(p, W_K) = \frac{- \llbracket v \rrbracket + \llbracket p \rrbracket \frac{v^2}{a^2}}{2\sqrt{- \llbracket p \rrbracket \llbracket v \rrbracket}} > 0, \tag{3.30}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}p^2} f_K(p, W_K) = -\frac{1}{4(- \llbracket p \rrbracket \llbracket v \rrbracket)^{3/2}} \left(-4 \llbracket p \rrbracket^2 \llbracket v \rrbracket \frac{v^3}{a^4} \mathcal{G} + \left(\llbracket p \rrbracket \frac{v^2}{a^2} - \llbracket v \rrbracket \right)^2 \right) < 0$$

For a rarefaction wave we yield

$$\frac{\mathrm{d}}{\mathrm{d}p} f_K(p, W_K) = \frac{v(p)}{a(p)} > 0, \tag{3.31}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}p^2} f_K(p, W_K) = -\frac{v(p)^2}{a(p)^3} \mathcal{G} < 0$$

Combining (3.30) with (3.31) gives

$$\frac{\mathrm{d}}{\mathrm{d}p} f(p, W_L, W_R) > 0 \quad \text{and} \quad \frac{\mathrm{d}^2}{\mathrm{d}p^2} f(p, W_L, W_R) < 0. \tag{3.32}$$

Using the asymptotic behavior of $v(p)$ gives

$$f(p, W_L, W_R) \overset{p\to 0}{\to} -\infty \quad \text{and} \quad f(p, W_L, W_R) \overset{p\to\infty}{\to} +\infty \tag{3.33}$$

and hence we have a unique root which determines the solution of our system.

3.2 Solution at the Interface

The phase boundary separating the liquid and the vapor phase is a non-classical or under compressive shock, see [18] or [55] and references therein. Hence the Lax criterion alone will not give us a unique solution and we need a further relation at the interface. This equation is called *kinetic relation*. We use the kinetic relation derived by Dreyer et al. [23]. The kinetic relation is chosen such that the mass flux z is proportional to the jump term in the entropy inequality (3.5)

$$z \left[\!\left[g + e^{kin} \right]\!\right] \geq 0,$$

see also Remark 2.2.1. If we assume the vapor left to the liquid phase the kinetic relation reads

$$z = \tau p_V \left[\!\left[g + e^{kin} \right]\!\right] = \tau p_V [g_L - g_V + e_L^{kin} - e_V^{kin}]. \tag{3.34}$$

Otherwise we can use

$$z = -\tau p_V [g_L - g_V + e_L^{kin} - e_V^{kin}]. \tag{3.35}$$

In the following we will assume the first case. In this section we will prove that there exists a unique solution of the equations at the interface provided certain conditions hold. By this we mean that there exists a unique liquid (vapor) state for a prescribed vapor (liquid) state such that the following equations hold

$$\begin{aligned} [\![z]\!] &= 0, \\ -z [\![u]\!] + [\![p]\!] &= 0, \\ z &= \tau p_V \left[\!\left[g + e^{kin} \right]\!\right]. \end{aligned}$$

Here e^{kin} denotes the *kinetic energy*. Furthermore we have for the so called *mobility* $0 < \tau \in \mathbb{R}$. Usually one uses

$$\tau = \frac{1}{\sqrt{2\pi}} \left(\frac{m}{kT_0} \right)^{\frac{3}{2}} \tag{3.36}$$

where m denotes the mass of a single molecule, k the Boltzmann constant and T_0 the fixed temperature, see [10, 23]. Using the jump conditions (3.3) and (3.4) we can rewrite (3.34) and obtain

$$z = \tau p_V \left[\!\left[g - \frac{1}{2} p(v_L + v_V) \right]\!\right]. \tag{3.37}$$

Furthermore we can combine the jump conditions and obtain

$$[\![p]\!] + z^2 [\![v]\!] = 0. \tag{3.38}$$

Together with the EOS and (3.37) equation (3.38) is a single equation for one unknown given one state at the phase boundary. For example we will prescribe the vapor pressure and then obtain the liquid pressure as the solution of equation (3.38). In the following we will assume as before that $\gamma_V \geq 0$ and $\mathcal{G}_K > 0$, $K \in \{V, L\}$. From the mathematical point of view we need further assumptions to solve the problem. A discussion will be given later on and it will turn out that these assumptions are rather liberal from a physical point of view, see Subsection 3.5.1. In the following we need the quotient of the specific volumes to be uniformly bounded as well as the corresponding sound speeds

$$\begin{aligned} &0 < \frac{v_L}{v_V} \leq \alpha < 1, \quad 0 < \frac{v_L}{v_V}\frac{a_V}{a_L} \leq \alpha\beta < 1, \quad \tau(1-\alpha)^2 a_V^3 < \gamma_V \quad \text{and} \\ &0 < p_V \leq \sigma_{max} p_0 \quad \text{with} \quad \sigma_{max} = \frac{1 + \sqrt{11 - 6\alpha}}{2}. \end{aligned} \tag{3.39}$$

Remark 3.2.1. *The specific volume and the speed of sound depend on the pressure but for convenience we often will not write out this dependence explicitly.*

Now we can state one of the main results of this work.

Theorem 3.2.2 (Existence and Uniqueness of a Solution at the Interface)**.** *For two phases each described by a thermodynamic consistent equation of state meeting the requirements (3.39) and*

$$-a_V/v_V \leq z \leq a_L/v_L$$

exists a unique solution of equation (3.38). Furthermore the mass flux z is uniquely defined. The liquid pressure can be written as a function of the vapor pressure and has the following properties

$$p_L^* = \varphi(p_V^*) \geq p_V^*, \ \varphi(p_0) = p_0, \ \frac{\mathrm{d}\varphi(p_V^*)}{\mathrm{d}p_V^*} > 0$$

In the remaining part of this section we will give the proof of this theorem.

3.2.1 Proof

The proof of Theorem 3.2.2 is based on the *implicit function theorem*. The main steps are the following

(i) We define a function $f(p_V, p_L)$, see (3.40), which we will analyze and where the roots correspond to the solution of (3.38).

(ii) The local existence of an admissible root, see Definition 3.2.3, for the equilibrium case (p_0, p_0) is given in Remark 3.2.4.

(iii) Lemma 3.2.7 and Lemma 3.2.8 state that the first order derivatives of $f(p_V, p_L)$ each have a sign for an admissible solution.

(iv) Uniqueness is shown in Lemma 3.2.11 and global existence is stated and proven in Lemma 3.2.12.

Replacing z in (3.38) using (3.37) we obtain

$$[\![p]\!] + \left(\tau p_V \left[\!\!\left[g - \frac{1}{2}p(v_L + v_V) \right]\!\!\right]\right)^2 [\![v]\!] = 0.$$

According to this equation we define the following functions

$$\begin{aligned} h(p_V, p_L) &:= \tau \left[\!\!\left[g - \frac{1}{2}p(v_L + v_V) \right]\!\!\right] \\ &= \tau \left[g_L(p_L) - g_V(p_V) - \frac{1}{2}(p_L - p_V)(v_L(p_L) + v_V(p_V)) \right], \\ f(p_V, p_L) &:= [\![p]\!] + (p_V h(p_V, p_L))^2 [\![v]\!] . \end{aligned} \tag{3.40}$$

Obviously every root of (3.40) is a solution of (3.38) and we easily see

$$0 = f(p_V^*, p_L^*) \overset{[\![v]\!]<0}{\Rightarrow} [\![p]\!] \geq 0. \tag{3.41}$$

Let us furthermore define the following

Definition 3.2.3 (Admissible Solution)**.** *Let* (p_V^*, p_L^*) *be a solution of* $f(p_V^*, p_L^*) = 0$*. We say this solution is admissible if further the following inequalities hold*

$$-\frac{a_V(p_V^*)}{v_V(p_V^*)} \leq p_V^* h(p_V^*, p_L^*) \leq \frac{a_L(p_L^*)}{v_L(p_L^*)}.$$

The quantities a_K and v_K with $K \in \{L, V\}$ are functions of the pressure as already mentioned in Remark 3.2.1. Thus the bounds are evaluated at the pressures (p_V^*, p_L^*) which solve $f(p_V^*, p_L^*) = 0$.

Remark 3.2.4. *It is immediately verified that a solution* $f(p_V^*, p_L^*) = 0$ *with* $p_V^* = p_L^* =: p_0$ *implies equilibrium* $g_L(p_L^*) = g_V(p_V^*)$ *and vice versa. Thus we further obtain*

$$f(p_0, p_0) = 0,\ \partial_{p_V} f(p_0, p_0) = -1,\ \partial_{p_L} f(p_0, p_0) = 1 \quad \textit{with} \quad p_0 h(p_0, p_0) = 0. \tag{3.42}$$

Hence there exists a neighborhood of $p_V = p_0$ *such that (3.38) implicitly defines a function* $p_L = \varphi(p_V)$ *with* $\varphi'(p_V) > 0$*. Additionally* (p_0, p_0) *is an admissible solution with* $z = 0$*.*

Lemma 3.2.5. *The function* $h(p_V, p_L)$ *is strictly monotonically decreasing in* p_L *under the given assumptions, i.e.*

$$\partial_{p_L} h(p_V, p_L) < 0.$$

Proof: We obtain for the partial derivative of $h(p_V, p_L)$ using $(3.6)_2$

$$\partial_{p_L} h(p_V, p_L) = \frac{\tau}{2}\left\{ [\![v]\!] + [\![p]\!] \frac{v_L^2}{a_L^2} \right\}.$$

Let us consider $[\![p]\!] \geq 0$ since it is the only relevant case and the statement is obvious for $[\![p]\!] \leq 0$ anyway. Since $\mathcal{G}_L > 0$ we yield for the second partial derivative with respect to p_L using $(3.6)_2$ and (3.11)

$$\partial_{p_L}^2 h(p_V, p_L) = -\tau\, [\![p]\!] \frac{v_L^3}{a_L^4} \mathcal{G}_L < 0.$$

For $p_L = p_V$ we know that the Lemma is true and if we increase p_L the function is decreasing. Keep in mind that we have $[\![p]\!] > 0$. Hence we conclude $\partial_{p_L} h(p_V, p_L) < 0$. □

Corollary 3.2.6. *Every root of (3.40) with $z > 0$ is admissible.*

Proof: Using Lemma 3.2.5 one obtains for $f(p_V^*, p_L^*) = 0$ with $z = p_V^* h(p_V^*, p_L^*)$

$$z^2 = \left(p_V^* h(p_V^*, p_L^*)\right)^2 \overset{(3.40)}{=} -\frac{[\![p^*]\!]}{[\![v(p^*)]\!]} \overset{\text{Lem. 3.2.5}}{<} \frac{a_L^2}{v_L^2}.$$

□

Lemma 3.2.7. *Let (p_V^*, p_L^*) be an admissible solution of $f(p_V^*, p_L^*) = 0$. Then the following inequality holds*

$$\partial_{p_L} f(p_V^*, p_L^*) > 0.$$

Proof: For the equilibrium solution (3.42) the stated relation is obvious. Let us consider $p_V^* h(p_V^*, p_L^*) > 0$. Using Lemma 3.2.5 and $[\![v]\!] < 0$ we have

$$\partial_{p_L} f(p_V^*, p_L^*) = 1 + 2\underbrace{(p_V^* h(p_V^*, p_L^*))}_{>0}\underbrace{(p_V^* \partial_{p_L} h(p_V^*, p_L^*))\,[\![v]\!]}_{>0} - \underbrace{(p_V^* h(p_V^*, p_L^*))^2 \frac{v_L^2}{a_L^2}}_{<1} > 0.$$

It remains to prove the Lemma for the case $p_V^* h(p_V^*, p_L^*) < 0$. We can write

$$\begin{aligned}
\partial_{p_L} f(p_V^*, p_L^*) &= 1 + 2(p_V^* h(p_V^*, p_L^*))(p_V^* \partial_{p_L} h(p_V^*, p_L^*))\,[\![v]\!] - (p_V^* h(p_V^*, p_L^*))^2 \frac{v_L^2}{a_L^2} \\
&= 1 + \tau p_V^* (p_V^* h(p_V^*, p_L^*))\,[\![v]\!]^2 \left(1 - (p_V^* h(p_V^*, p_L^*))^2 \frac{v_L^2}{a_L^2}\right) - (p_V^* h(p_V^*, p_L^*))^2 \frac{v_L^2}{a_L^2} \\
&= \left(1 - (p_V^* h(p_V^*, p_L^*))^2 \frac{v_L^2}{a_L^2}\right)\left(1 + \tau p_V^* (p_V^* h(p_V^*, p_L^*))\,[\![v]\!]^2\right).
\end{aligned}$$

The first term is positive, because of $-a_V/v_V \le p_V^* h(p_V^*, p_L^*) < 0$ and $a_V^2/v_V^2 < a_L^2/v_L^2$. For the second term we have

$$0 < 1 + \tau p_V^* (p_V^* h(p_V^*, p_L^*))\,[\![v]\!]^2 \quad \overset{p_V^* h(p_V^*, p_L^*) < 0}{\Leftrightarrow} \quad \tau < -\frac{1}{p_V^* (p_V^* h(p_V^*, p_L^*))\,[\![v]\!]^2}.$$

Indeed we obtain

$$\begin{aligned}
-&\frac{1}{p_V^*(p_V^* h(p_V^*,p_L^*))\,[\![v]\!]^2} > \frac{v_V}{p_V^* a_V\,[\![v]\!]^2} \\
=&\frac{1}{p_V^* v_V a_V\left(\dfrac{v_L}{v_V}-1\right)^2} \overset{(3.39)_1}{\geq} \frac{\gamma_V}{(1-\alpha)^2 a_V^3} \overset{(3.39)_3}{>} \tau.
\end{aligned}$$

This proves the Lemma. □

Lemma 3.2.8. *Let* (p_V^*, p_L^*) *be an admissible solution of* $f(p_V^*, p_L^*) = 0$. *Then the following inequality holds*

$$\partial_{p_V} f(p_V^*, p_L^*) < 0. \tag{3.43}$$

Proof: Since we have $f(p_V^*, p_L^*) = 0$ we can write for $\partial_{p_V} h(p_V^*, p_L^*)$

$$\partial_{p_V} h(p_V^*, p_L^*) = \frac{\tau}{2}\left\{[\![v]\!] + [\![p]\!]\frac{v_V^2}{a_V^2}\right\} \overset{(3.40)}{=} \frac{\tau}{2}[\![v]\!]\left(1-(p_V^* h(p_V^*, p_L^*))^2\frac{v_V^2}{a_V^2}\right) \tag{3.44}$$

and hence we conclude

$$\partial_{p_V} h(p_V^*, p_L^*)\begin{cases} <0, & (p_V^* h(p_V^*, p_L^*))^2 < \dfrac{a_V^2}{v_V^2}, \\ \\ \geq 0, & (p_V^* h(p_V^*, p_L^*))^2 \geq \dfrac{a_V^2}{v_V^2}. \end{cases}$$

In the following we will discuss three cases depending on $p_V^* h(p_V^*, p_L^*)$.

First Case: We discuss the case where $-a_V/v_V \leq p_V^* h(p_V^*, p_L^*) \leq 0$. It is obvious to see

$$\partial_{p_V} f(p_V^*, p_L^*) = \left\{\begin{matrix} -1 & , & p_V^* h(p_V^*, p_L^*) = 0, \\ 2\dfrac{a_V^2}{p_V^* v_V^2}[\![v]\!] & , & p_V^* h(p_V^*, p_L^*) = -\dfrac{a_V}{v_V} \end{matrix}\right\} < 0.$$

In between we have $-a_V/v_V < p_V^* h(p_V^*, p_L^*) < 0$ and so all together

$\partial_{p_V} f(p_V^*, p_L^*) = \dots$

$$= -1 + 2\underbrace{(p_V^* h(p_V^*, p_L^*))}_{<0}\underbrace{(h(p_V^*, p_L^*) + p_V^*\partial_{p_V} h(p_V^*, p_L^*))}_{<0}[\![v]\!] + \underbrace{(p_V^* h(p_V^*, p_L^*))^2\frac{v_V^2}{a_v^2}}_{<1} < 0.$$

For $0 < p_V^* h(p_V^*, p_L^*) < a_L/v_L$ we split the proof into two parts. First we discuss the interval up to a_V/v_V and then the remaining part smaller than a_L/v_L.

Second Case: Using $0 < p_V^* h(p_V^*, p_L^*) \leq a_V/v_V$ we obtain

$$\begin{aligned}
&\partial_{p_V} f(p_V^*, p_L^*) = \dots \\
&= \; -1 + 2(p_V^* h(p_V^*, p_L^*))(h(p_V^*, p_L^*) + p_V^* \partial_{p_V} h(p_V^*, p_L^*)) [\![v]\!] + (p_V^* h(p_V^*, p_L^*))^2 \frac{v_V^2}{a_V^2} \\
&\overset{(3.44)}{=} \underbrace{\left(1 - (p_V^* h(p_V^*, p_L^*))^2 \frac{v_V^2}{a_V^2}\right)}_{\geq 0} \left(\tau p_V^{*2} h(p_V^*, p_L^*) [\![v]\!]^2 - 1\right) + \underbrace{2 p_V^* (h(p_V^*, p_L^*))^2 [\![v]\!]}_{<0}.
\end{aligned}$$

For the second term we obtain (as before in the proof of Lemma 3.2.7)

$$0 > \tau p_V^* (p_V^* h(p_V^*, p_L^*)) [\![v]\!]^2 - 1 \quad \overset{p_V^* h(p_V^*, p_L^*) > 0}{\Leftrightarrow} \quad \tau < \frac{1}{p_V^* (p_V^* h(p_V^*, p_L^*)) [\![v]\!]^2}.$$

and again we have

$$\begin{aligned}
\frac{1}{p_V^* (p_V^* h(p_V^*, p_L^*)) [\![v]\!]^2} &\geq \frac{v_V}{p_V^* a_V [\![v]\!]^2} \\
&= \frac{1}{p_V^* v_V a_V \left(\frac{v_L}{v_V} - 1\right)^2} \overset{(3.39)_1}{\geq} \frac{\gamma_V}{(1-\alpha)^2 a_V^3} \overset{(3.39)_3}{>} \tau.
\end{aligned}$$

This proves the Lemma for $0 < p_V^* h(p_V^*, p_L^*) \leq a_V/v_V$.

Third Case: We discuss $a_V/v_V < p_V^* h(p_V^*, p_L^*) < a_L/v_L$ and rewrite $\partial_{p_V} f(p_V^*, p_L^*)$

$$\begin{aligned}
&\partial_{p_V} f(p_V^*, p_L^*) = \dots \\
&= -1 + 2(p_V^* h(p_V^*, p_L^*))(h(p_V^*, p_L^*) + p_V^* \partial_{p_V} h(p_V^*, p_L^*)) [\![v]\!] + (p_V^* h(p_V^*, p_L^*))^2 \frac{v_V^2}{a_V^2} \\
&= -\left(1 - (p_V^* h(p_V^*, p_L^*))^2 \frac{v_V^2}{a_V^2}\right) + 2(p_V^* h(p_V^*, p_L^*))(p_V^* \partial_{p_V^*} h(p_V^*, p_L^*)) [\![v]\!] \\
&+ 2 p_V^* h(p_V^*, p_l^*)^2 [\![v]\!]
\end{aligned}$$

and further obtain using equation (3.44)

$$\begin{aligned}
&\partial_{p_V} f(p_V^*, p_L^*) = \dots \\
&= -\frac{2}{\tau \llbracket v \rrbracket} \partial_{p_V} h(p_V^*, p_L^*) + p_V^* h(p_V^*, p_L^*))(p_V^* \partial_{p_V^*} h(p_V^*, p_L^*)) \llbracket v \rrbracket + 2 p_V^* h(p_V^*, p_l^*)^2 \llbracket v \rrbracket \\
&= \underbrace{-\frac{2}{\tau \llbracket v \rrbracket} \partial_{p_V} h(p_V^*, p_L^*)}_{>0} \underbrace{\left(1 - \tau p_V^* \llbracket v \rrbracket^2 p_V^* h(p_V^*, p_L^*)\right)}_{\overset{(3.39)}{<0}} + \underbrace{2 p_V^* h(p_V^*, p_l^*)^2 \llbracket v \rrbracket}_{<0} < 0.
\end{aligned}$$

This ends the proof. □

Corollary 3.2.9 (Monotonicity of the Implicit Function). *Let* (p_V^*, p_L^*) *be an admissible solution* $f(p_V^*, p_L^*) = 0$. *Then there exists a function* φ *with* $p_L^* = \varphi(p_V^*)$ *which is strictly monotonically increasing, i.e.* $\varphi'(p_V^*) > 0$.

Proof: This follows using the implicit function theorem together with Lemma 3.2.7 and 3.2.8. □

Corollary 3.2.10. *During a condensation process both pressures are larger than the saturation pressure*

$$p_0 < p_V < p_L$$

whereas during evaporation both pressures are smaller than the saturation pressure

$$p_V < p_L < p_0.$$

Proof: This follows from Corollary 3.2.9 and $p_L(p_0) = p_0$. □

Lemma 3.2.11 (Uniqueness). *Let* (p_V^*, p_L^*) *be an admissible solution of* $f(p_V^*, p_L^*) = 0$. *Then this root is unique in the sense that for a given* p_V^* *the solution* p_L^* *is unique.*

Proof: First we assume that there exists a $p_L^{**} > p_L^*$ such that $f(p_V^*, p_L^{**}) = 0$. From Lemma 3.2.7 we know that $\partial_{p_L} f(p_V^*, p_L^*) > 0$. Hence we have (monotonicity argument) $\partial_{p_L} f(p_V^*, p_L^{**}) \leq 0$. Therefore we have

$$\underbrace{p_V^* h(p_V^*, p_L^{**}) < -\frac{a_V}{v_V}}_{\mathbf{I}} \quad \dot{\vee} \quad \underbrace{p_V^* h(p_V^*, p_L^{**}) > \frac{a_L}{v_L}}_{\mathbf{II}} \tag{3.45}$$

otherwise we would meet the requirements of Lemma 3.2.7. Since $p_V^* h(p_V^*, p_L^*) \leq a_L/v_L$ and Lemma 3.2.5 we can exclude **II**. Assuming **I** is true we have that the root (p_V^*, p_L^{**}) itself is not admissible and every possible further root with $p_L > p_L^{**}$ would also fulfill relation **I** due to Lemma 3.2.5 and thus is not admissible.

Now we assume that there exists a $p_L^{**} < p_L^*$ such that $f(p_V^*, p_L^{**}) = 0$. As in the first case we have the two possibilities (3.45). The arguments are now quite analogue to the first case. We can exclude **I** since

$$-\frac{a_V}{v_V} \leq p_V^* h(p_V^*, p_L^*) < p_V^* h(p_V^*, p_L^{**}).$$

Therefore relation **II** must hold and p_L^{**} is no admissible root. Due to Lemma 3.2.5 every further solution $p_L < p_L^{**}$ also fulfills **II**. This proves uniqueness.

□

Lemma 3.2.12 (Global Existence)**.** *For every* $p_V^* \in [0, \sigma_{max} p_0]$ *exists a* $p_L^* \in [p_V^*, \infty)$ *such that* (p_V^*, p_L^*) *is an admissible root of* $f(p_V^*, p_L^*) = 0$.

Proof: We already have local existence in a neighborhood of (p_0, p_0) due to the implicit function theorem. In the following we discriminate the cases depending on whether p_V is smaller or larger than the saturation pressure p_0.

First Case ($\mathbf{0 \leq p_V < p_0}$): Assume that there exists a $p_V < p_0$ such that there exists *no* p_L with $f(p_V, p_L) = 0$. Using the above results we know that there exists an admissible root (p_V^*, p_L^*) in the neighborhood of (p_0, p_0) and due to monotonicity/continuity a further root $p_V < \bar{p}_V < p_V^*$ and $\bar{p}_L$ such that

$$f(\bar{p}_V, \bar{p}_L) = 0 \ \wedge \ \partial_{p_L} f(\bar{p}_V, \bar{p}_L) = 0.$$

Hence this root is *not* admissible due to Lemma 3.2.7. On the other hand we have, due to the behavior of the function $h(p_V, p_L)$ in (p_0, p_0) and the fact that

$$f(p_V, p_L) = 0 \ \wedge \ h(p_V, p_L) = 0 \quad \Leftrightarrow \quad [\![p]\!] = 0,$$

that $h(\bar{p}_V, \bar{p}_L) > 0$ for $\bar{p}_V < p_0$. Together with Corollary 3.2.6 this gives

$$0 < \bar{p}_V h(\bar{p}_V, \bar{p}_L) \leq \frac{a_L}{v_L}.$$

This contradicts the above statement that the root $\bar{p}_V$ is not admissible. Therefore the nonexistence assumption is wrong and we have global existence for $0 \leq p_V < p_0$.

Second Case ($\mathbf{p_0 < p_V \leq \sigma_{max} p_0}$): The idea is again to show, that there exists no $p_0 < p_V^* \leq \sigma_{max} p_0$ such that

$$f(p_V^*, p_L^*) = 0 \;\wedge\; \partial_{p_L} f(p_V^*, p_L^*) = 0. \tag{3.46}$$

Let us assume we have (p_V^*, p_L^*) such that the above relation holds. From that we can conclude

$$\begin{aligned}
&\partial_{p_L} f(p_V^*, p_L^*) = 0 \\
&\Leftrightarrow \\
&\left(p_V^* h(p_V^*, p_L^*)\right)^2 = \left(1 + 2(p_V^* h(p_V^*, p_L^*))(p_V^* \partial_{p_L} h(p_V^*, p_L^*)) \llbracket v \rrbracket\right) \frac{a_L^2}{v_L^2}.
\end{aligned}$$

Inserting this expression in $0 = f(p_V^*, p_L^*)$ gives

$$\begin{aligned}
0 = f(p_V^*, p_L^*) &= \llbracket p \rrbracket + \left(p_V^* h(p_V^*, p_L^*)\right)^2 \llbracket v \rrbracket \\
&= \llbracket p \rrbracket + \left(1 + 2(p_V^* h(p_V^*, p_L^*))(p_V^* \partial_{p_L} h(p_V^*, p_L^*)) \llbracket v \rrbracket\right) \frac{a_L^2}{v_L^2} \llbracket v \rrbracket \\
&= \llbracket p \rrbracket + \llbracket v \rrbracket \frac{a_L^2}{v_L^2} + 2(p_V^* h(p_V^*, p_L^*))(p_V^* \partial_{p_L} h(p_V^*, p_L^*)) \llbracket v \rrbracket^2 \\
&= \frac{2}{\tau} \frac{a_L^2}{v_L^2} \partial_{p_L} h(p_V^*, p_L^*) + 2(p_V^* h(p_V^*, p_L^*))(p_V^* \partial_{p_L} h(p_V^*, p_L^*)) \llbracket v \rrbracket^2 \\
&= \frac{2}{\tau} \partial_{p_L} h(p_V^*, p_L^*) \frac{a_L^2}{v_L^2} \left(1 + \tau \, {p_V^*}^2 \, h(p_V^*, p_L^*) \llbracket v \rrbracket^2\right)
\end{aligned}$$

We define the function

$$H(p_V, p_L) := 1 + \tau p_V^2 h(p_V, p_L) \llbracket v \rrbracket^2 .$$

Due to Lemma 3.2.5 we have $H(p_V^*, p_L^*) = 0$ and hence

$$p_V^* h(p_V^*, p_L^*) = -\frac{1}{\tau p_V^* \llbracket v \rrbracket^2}. \tag{3.47}$$

Further we can rewrite $\partial_{p_L} f(p_V, p_L)$ in terms of $H(p_V, p_L)$, i.e.

$$\begin{aligned}\partial_{p_L} f(p_V, p_L) &= \dots \\ &= -\frac{v_L^2}{\left(\tau p_V a_L [\![v]\!]^2\right)^2}(H(p_V, p_L) - 1)^2 + \left(1 + \frac{[\![p]\!]}{[\![v]\!]}\frac{v_L^2}{a_L^2}\right)(H(p_V, p_L) - 1) + 1.\end{aligned}$$

From this we immediately yield

$$\begin{aligned}&H(p_V, p_L) = \partial_{p_L} f(p_V, p_L) \\ &\Leftrightarrow \\ &0 = (H(p_V, p_L) - 1)\left(-\frac{v_L^2}{\left(\tau p_V a_L [\![v]\!]^2\right)^2}(H(p_V, p_L) - 1) + \frac{[\![p]\!]}{[\![v]\!]}\frac{v_L^2}{a_L^2}\right).\end{aligned}$$

For the considered root (p_V^*, p_L^*) we can exclude the first case since $H(p_V^*, p_L^*) = 1$ if and only if $p_V^* h(p_V^*, p_L^*) = 0$. Hence we further look at the second term which must vanish for (p_V^*, p_L^*) and obtain

$$H(p_V^*, p_L^*) = \left(\tau p_V^* [\![v]\!]^2\right)^2 \frac{[\![p]\!]}{[\![v]\!]} + 1 \quad \Leftrightarrow \quad p_V^* h(p_V^*, p_L^*) = \tau p_V^* [\![p]\!] [\![v]\!] . \tag{3.48}$$

Summing up we can state that there are two conditions (3.47) and (3.48) which need to be true for (p_V^*, p_L^*) when (3.46) holds. For equation (3.47) we easily verify

$$p_V^* h(p_V^*, p_L^*) = -\frac{1}{\tau p_V^* [\![v]\!]^2} \overset{(3.39)_1}{\leq} -\frac{1}{\tau p_V^* v_V^2 (1-\alpha)^2} \overset{(3.39)_3}{<} -\frac{a_V}{v_V}. \tag{3.49}$$

Now we investigate (3.48) and prove that this implies $p_V^* h(p_V^*, p_L^*) > -a_V/v_V$. This would contradict (3.49) and hence finish the proof.
First we introduce the following functions for fixed p_V^*

$$\begin{aligned}F(p_L) &:= p_V^* h(p_V^*, p_L), & F'(p_L) &= p_V^* \partial_{p_L} h(p_V^*, p_L), \\ G(p_L) &:= \tau p_V^* [\![p]\!] [\![v]\!] , & G'(p_L) &= \tau p_V^* \left\{ [\![v]\!] - [\![p]\!] \frac{v_L^2}{a_L^2} \right\}.\end{aligned}$$

We immediately verify for all $p_L \geq p_V^*$

$$G'(p_L) < F'(p_L) < 0.$$

Furthermore we have

$$G(p_V^*) = 0 \overset{p_V^*>p_0}{>} F(p_V^*) = p_V^* h(p_V^*, p_V^*) = \tau p_V^* \left\llbracket g(p_V^*) \right\rrbracket .$$

Surely there is a $\bar{p}_L > p_V^*$ such that

$$G(\bar{p}_L) = -\frac{a_V}{v_V} \quad \text{with} \quad \bar{p}_L = p_V^* - \frac{a_V}{\tau p_V^* v_V \llbracket v \rrbracket} \leq p_V^* + \frac{a_V}{\tau p_V^* v_V^2 (1-\alpha)}. \tag{3.50}$$

Now we investigate $F(\bar{p}_L)$ and obtain

$$\begin{aligned} F(\bar{p}_L) &= p_V^* h(p_V^*, \bar{p}_L) = \tau p_V^* \left\{ \llbracket g \rrbracket - \frac{1}{2} \llbracket p \rrbracket (v_L + v_V) \right\} \\ &\overset{(3.50)}{=} \tau p_V^* (\llbracket g \rrbracket - v_V \llbracket p \rrbracket) + \frac{1}{2}\frac{a_V}{v_V}. \end{aligned}$$

We have for $p_V^* = \sigma p_0$ with $\sigma \in [1, \sigma_{max}]$

$$\begin{aligned} \tau p_V^* (\llbracket g \rrbracket - v_V \llbracket p \rrbracket) &\overset{g_L(\bar{p}_L) > g_L(p_V^*)}{>} \tau p_V^* \left(\left\llbracket g(p_V^*) \right\rrbracket - v_V \llbracket p \rrbracket \right) \\ &\overset{(3.50)}{\geq} \tau p_V^* \left\{ \left\llbracket g(p_V^*) \right\rrbracket - \frac{a_V}{\tau p_V^* v_V (1-\alpha)} \right\} = \tau p_V^* \left\llbracket g(p_V^*) \right\rrbracket - \frac{a_V}{v_V(1-\alpha)} \\ &\overset{\text{Taylor}}{\geq} \tau p_V^* \llbracket v(p_0) \rrbracket (p_V^* - p_0) - \frac{a_V}{v_V(1-\alpha)} \\ &> \frac{v_V(p_0)}{a_V(p_0) \llbracket v(p_0) \rrbracket} \sigma(\sigma-1) p_0 - \frac{a_V}{v_V(1-\alpha)} \\ &\geq -\frac{a_V(p_0)}{v_V(p_0)} \frac{\sigma(\sigma-1)}{1-\alpha} - \frac{a_V}{v_V(1-\alpha)} \\ &\overset{\frac{\mathrm{d}}{\mathrm{d}p}\frac{a(p)}{v(p)}>0}{>} -\frac{a_V(p_V^*)}{v_V(p_V^*)} \frac{\sigma(\sigma-1)-1}{1-\alpha} \\ &\overset{\sigma \leq \sigma_{max}}{\geq} -\frac{3}{2}\frac{a_V}{v_V}. \end{aligned}$$

This gives us $F(\bar{p}_L) > G(\bar{p}_L)$ and so there exists a $p_L^{**} \in (p_V^*, \bar{p}_L)$ such that

$$F(p_L^{**}) = G(p_L^{**}) > -\frac{a_V}{v_V}. \tag{3.51}$$

Thus condition (3.48) contradicts the first condition (3.47). Hence there exists *no* (p_V^*, p_L^*) such that relation (3.46) holds. This implies global existence for all $p_0 < p_V \leq \sigma_{max} p_0$ and finishes the proof. □

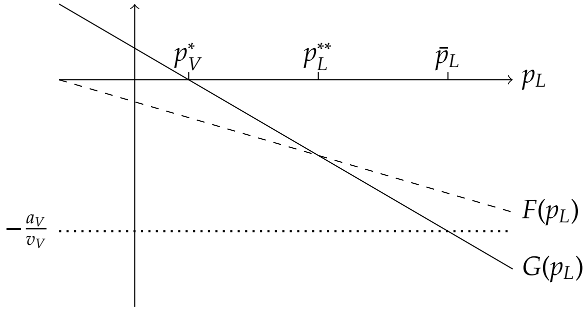

Figure 3.1: Idea for the contradiction argument

3.3 Solution of the Two Phase Riemann Problem

In this section we want to solve the Riemann problem. Therefore we follow the strategy of constructing *wave curves* and obtain the solution as the intersection of the wave curves, as for example done in [60, 78]. Due to the phase boundary we have an additional term, but we still want to show uniqueness of a solution to the Riemann problem. Hence we need a further monotonicity argument which we will prove in the following.
To this end we additionally need bounds for the dimensionless speed of sound γ_V and γ_L. We distinguish two relevant cases, each with an appropriate condition needed to prove monotonicity. This is necessary especially for EOS (or equivalently fluids) near the critical point, e.g. *van der Waals* EOS. Further these conditions show that the dimensionless quantities are not independent of each other. We consider the following relevant cases

$$\begin{aligned}
&\textbf{(I)} \begin{cases} \gamma_V & \leq 1 \quad \text{and} \quad 1 \leq \gamma_L \quad \text{with,} \\ \dfrac{1}{\gamma_L} & \geq 1 + \dfrac{\varepsilon(\gamma_V)}{\alpha}. \end{cases} \\
&\textbf{(II)} \begin{cases} \gamma_V & < 1 \quad \text{and} \quad \gamma_L < 1 \quad \text{with,} \\ \alpha & \leq \dfrac{1 - \frac{1}{\gamma_V}}{1 - \frac{1}{\gamma_L}} \quad \text{and} \quad \varepsilon(\gamma_V) \leq 0. \end{cases}
\end{aligned} \tag{3.52}$$

The quantity $\varepsilon(\gamma_V)$ is defined as follows, using all quantities as introduced before,

$$\varepsilon(\gamma_V) := \frac{1}{\gamma_V} - 1 - \frac{\tau a_V^3}{\gamma_V^2}(1-\alpha)^2\left(1-(\alpha\beta)^2\right). \tag{3.53}$$

So far we proved in Section 3.2 that there exists a unique solution of the jump conditions at the interface. Furthermore we can express the pressure in the liquid phase as a strictly monotone increasing function of the vapor pressure

$$p_L^* = \varphi(p_V^*) \quad \text{with} \quad \varphi'(p_V^*) > 0.$$

Lemma 3.3.1. *Given the requirements (3.39) and (3.52). For an admissible solution $f(p_V^*, p_L^*) = 0$ the following monotonicity holds*

$$\frac{\mathrm{d}}{\mathrm{d}p_V}\left(p_V^* h(p_V^*, p_L^*) [\![v]\!]\right) \geq 0.$$

Proof: We have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}p_V}\left(p_V^* h(p_V^*, p_L^*) [\![v]\!]\right) &= \partial_{p_V}\left(p_V^* h(p_V^*, p_L^*) [\![v]\!]\right) + \partial_{p_L}\left(p_V^* h(p_V^*, p_L^*) [\![v]\!]\right)\varphi'(p_V^*)\\ &= \left(h(p_V^*, p_L^*) + p_V^*\partial_{p_V} h(p_V^*, p_L^*)\right) [\![v]\!] + p_V^* h(p_V^*, p_L^*)\frac{v_V^2}{a_V^2}\\ &\quad + \left\{p_V^*\partial_{p_L} h(p_V^*, p_L^*) [\![v]\!] - p_V^* h(p_V^*, p_L^*)\frac{v_L^2}{a_L^2}\right\}\varphi'(p_V^*).\end{aligned}$$

For (p_0, p_0) the statement is obvious and hence we assume $p_V^* h(p_V^*, p_L^*) \neq 0$ from now on. Hence we can write

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}p_V}\left(p_V^* h(p_V^*, p_L^*) [\![v]\!]\right) = \dots\\ &= \frac{1}{2p_V^* h(p_V^*, p_L^*)}\left(\partial_{p_V} f(p_V^*, p_L^*) + 1\right) + \frac{1}{2}p_V^* h(p_V^*, p_L^*)\frac{v_V^2}{a_V^2}\\ &+ \left\{\frac{1}{2p_V^* h(p_V^*, p_L^*)}\left(\partial_{p_L} f(p_V^*, p_L^*) - 1\right) - \frac{1}{2}p_V^* h(p_V^*, p_L^*)\frac{v_L^2}{a_L^2}\right\}\varphi'(p_V^*).\end{aligned}$$

Multiplication with $\partial_{p_L} f(p_V^*, p_L^*) > 0$ and use of

$$\varphi'(p_V^*) = -\frac{\partial_{p_V} f(p_V^*, p_L^*)}{\partial_{p_L} f(p_V^*, p_L^*)}.$$

gives

$$\begin{aligned}
&\partial_{p_L} f(p_V^*, p_L^*) \frac{\mathrm{d}}{\mathrm{d}p_V} \left(p_V^* h(p_V^*, p_L^*) [\![v]\!] \right) = \dots \\
&= \left\{ \frac{1}{2p_V^* h(p_V^*, p_L^*)} (\partial_{p_V} f(p_V^*, p_L^*) + 1) + \frac{1}{2} p_V^* h(p_V^*, p_L^*) \frac{v_V^2}{a_V^2} \right\} \partial_{p_L} f(p_V^*, p_L^*) \\
&- \left\{ \frac{1}{2p_V^* h(p_V^*, p_L^*)} (\partial_{p_L} f(p_V^*, p_L^*) - 1) - \frac{1}{2} p_V^* h(p_V^*, p_L^*) \frac{v_L^2}{a_L^2} \right\} \partial_{p_V} f(p_V^*, p_L^*).
\end{aligned}$$

This can be reformulated to (see Appendix 9.1 for details)

$$\begin{aligned}
\partial_{p_L} f(p_V^*, p_L^*) \frac{\mathrm{d}}{\mathrm{d}p_V} \left(p_V^* h(p_V^*, p_L^*) [\![v]\!] \right) &= h(p_V^*, p_L^*) \left(v_L \left(1 - \frac{p_L^* v_L}{a_L^2} \right) - v_V \left(1 - \frac{p_V^* v_V}{a_V^2} \right) \right) \\
&+ \tau p_V [\![v]\!]^2 \left(1 - (p_V^* h(p_V^*, p_L^*))^4 \frac{v_V^2}{a_V^2} \frac{v_L^2}{a_L^2} \right).
\end{aligned}$$

Due to the bounds for the *EOS* we can show

$$\left(v_L \left(1 - \frac{p_L^* v_L}{a_L^2} \right) - v_V \left(1 - \frac{p_V^* v_V}{a_V^2} \right) \right) \geq 0.$$

and hence we can immediately verify the Lemma for

$$0 < p_V^* h(p_V^*, p_L^*) \leq \sqrt{\frac{a_V}{v_V} \frac{a_L}{v_L}}.$$

Now we want to prove the result for $0 > p_V^* h(p_V^*, p_L^*) \geq -a_V/v_V$.We have

$$\begin{aligned}
&h(p_V^*, p_L^*)\left(v_L\left(1-\frac{p_L^* v_L}{a_L^2}\right) - v_V\left(1-\frac{p_V^* v_V}{a_V^2}\right)\right) + \tau p_V^* [\![v]\!]^2 \left(1-(p_V^* h(p_V^*, p_L^*))^4 \frac{v_V^2}{a_V^2}\frac{v_L^2}{a_L^2}\right) \\
\geq \quad & -\frac{a_V}{p_V^* v_V}\left(v_L\left(1-\frac{1}{\gamma_L}\right) - v_V\left(1-\frac{1}{\gamma_V}\right)\right) + \tau p_V^* [\![v]\!]^2 \left(1-\frac{a_V^2}{v_V^2}\frac{v_L^2}{a_L^2}\right) \\
\geq \quad & -\frac{\gamma_V}{a_V}\left(v_L\left(1-\frac{1}{\gamma_L}\right) - v_V\left(1-\frac{1}{\gamma_V}\right)\right) + \tau v_V^2 p_V^* (1-\alpha)^2\left(1-(\alpha\beta)^2\right) \\
= \quad & -\frac{v_V}{a_V}\left(\frac{\gamma_V}{\gamma_L}\frac{v_L}{v_V}(\gamma_L - 1) + (1-\gamma_V)\right) + \tau v_V^2 p_V^* (1-\alpha)^2\left(1-(\alpha\beta)^2\right) \\
= \quad & -\frac{v_V}{a_V}\left(\frac{\gamma_V}{\gamma_L}\frac{v_L}{v_V}(\gamma_L - 1) + (1-\gamma_V) - \frac{\tau a_V^3}{\gamma_V}(1-\alpha)^2\left(1-(\alpha\beta)^2\right)\right) \qquad (+) \\
\overset{\gamma_L \geq 1}{\geq} \quad & -\frac{v_V}{a_V}\left(\alpha\frac{\gamma_V}{\gamma_L}(\gamma_L - 1) + (1-\gamma_V) - \frac{\tau a_V^3}{\gamma_V}(1-\alpha)^2\left(1-(\alpha\beta)^2\right)\right) \\
\geq \quad & \alpha\gamma_V\frac{v_V}{a_V}\left(\frac{1}{\gamma_L} - \left(1+\frac{\varepsilon(\gamma_V)}{\alpha}\right)\right) \\
\overset{(3.52)(\mathbf{I})}{\geq} \quad & 0.
\end{aligned}$$

Starting from (+) we obtain for the case $1 > \gamma$ for both phases

$$\begin{aligned}
& -\frac{v_V}{a_V}\left(\frac{\gamma_V}{\gamma_L}\frac{v_L}{v_V}(\gamma_L - 1) + (1-\gamma_V) - \frac{\tau a_V^3}{\gamma_V}(1-\alpha)^2\left(1-(\alpha\beta)^2\right)\right) \\
\geq \quad & -\frac{v_V}{a_V}\left(1-\gamma_V - \frac{\tau a_V^3}{\gamma_V}(1-\alpha)^2\left(1-(\alpha\beta)^2\right)\right) \\
= \quad & -\gamma_V\frac{v_V}{a_V}\varepsilon(\gamma_V) \\
\overset{(3.52)(\mathbf{II})}{\geq} \quad & 0.
\end{aligned}$$

It remains the case for

$$\sqrt{\frac{a_V}{v_V}\frac{a_L}{v_L}} < p_V^* h(p_V^*, p_L^*) < \frac{a_L}{v_L}.$$

In the subsequent Lemma 3.3.3 we will exclude this case and thus the proof of this Lemma is finished. □

Remark 3.3.2 (Assumptions on γ). *In Lemma 3.3.1 we only consider cases where $\gamma_V \in (0,1]$ for the vapor phase. As mentioned before the lower bound ensures hyperbolicity and thermodynamic stability. The upper bound is due to the fact, that we only consider pressures and temperatures* below *the critical point. To illustrate this we consider the* isothermal compressibility *κ_T which is defined as follows*

$$\kappa_T = -v\left(\frac{\partial v}{\partial p}\right)_T .$$

For real *gases κ_T can be expressed in terms of the pressure and the* compressibility *or* gas deviation factor *$\mathcal{Z}$ (not to confuse with the mass flux z used in this work), i.e.*

$$\kappa_T = \frac{1}{p} - \frac{1}{\mathcal{Z}}\left(\frac{\partial \mathcal{Z}}{\partial p}\right)_T .$$

Below the critical point the second term is negative for most gases (cf. [17, 48]) and hence

$$\kappa_T > \frac{1}{p} \quad \Leftrightarrow \quad \gamma_V = \frac{1}{p\kappa_T} < 1.$$

This property is reflected by nonlinear EOS such as the van der Waals *or* Dieterici *EOS. For an ideal gas the second term vanishes and we obtain $\gamma_V = 1$.*

Lemma 3.3.3. *Consider two phases such that the requirements (3.39) are fulfilled. Then there exists a maximal mass flux z_{max} such that for every admissible solution $f(p_V^*, p_L^*) = 0$ the following upper bound holds*

$$z_{max} \leq \sqrt{\frac{a_V}{v_V}\frac{a_L}{v_L}}.$$

Proof: Since $z(p_V) = 0$ if and only if $p_V = p_0$ and further $z(p_0)' < 0$ we can focus on vapor pressures smaller than p_0. We assume that

$$z_{max} > \sqrt{\frac{a_V}{v_V}\frac{a_L}{v_L}}.$$

Hence there exists a $\tilde{p} \in (0, p_0)$ such that

$$z(\tilde{p}) = \tilde{p}h(\tilde{p}, \varphi(\tilde{p})) = \sqrt{\frac{a_V}{v_V}\frac{a_L}{v_L}} \text{ and } z'(\tilde{p}) \leq 0.$$

This gives

$$
\begin{aligned}
0 \geq z'(\tilde{p}) &= \frac{1}{\tilde{p}}\sqrt{\frac{a_V}{v_V}\frac{a_L}{v_L}} + \tilde{p}\left(\partial_{p_V} h(\tilde{p},\varphi(\tilde{p})) + \partial_{p_L} h(\tilde{p},\varphi(\tilde{p}))\varphi'(\tilde{p})\right) \\
&= \frac{1}{\tilde{p}}\sqrt{\frac{a_V}{v_V}\frac{a_L}{v_L}} + \frac{\tau\tilde{p}}{2}[\![v]\!]\left(1 - \frac{a_L}{a_V}\frac{v_V}{v_L} + \left(1 - \frac{a_V}{a_L}\frac{v_L}{v_V}\right)\varphi'(\tilde{p})\right) \\
&= \underbrace{\frac{1}{\tilde{p}}\sqrt{\frac{a_V}{v_V}\frac{a_L}{v_L}}}_{>0} + \underbrace{\frac{\tau\tilde{p}}{2}[\![v]\!]\left(1 - \frac{a_V}{a_L}\frac{v_L}{v_V}\right)}_{<0}\left(\varphi'(\tilde{p}) - \frac{a_L}{a_V}\frac{v_V}{v_L}\right) \\
&\Rightarrow \xi := \varphi'(\tilde{p}) > \frac{a_L}{a_V}\frac{v_V}{v_L} \geq \frac{1}{\alpha\beta} \overset{(3.39)_2}{>} 1.
\end{aligned}
$$

Using the definition of $\varphi'(p_V)$ we obtain

$$
\begin{aligned}
&-\partial_{p_V} f(\tilde{p},\varphi(\tilde{p})) = \partial_{p_L} f(\tilde{p},\varphi(\tilde{p}))\xi \\
&\Leftrightarrow \\
&1 - 2\sqrt{\frac{a_V}{v_V}\frac{a_L}{v_L}}\left(\frac{1}{\tilde{p}}\sqrt{\frac{a_V}{v_V}\frac{a_L}{v_L}} + \tilde{p}\partial_{p_V} h(\tilde{p},\varphi(\tilde{p}))\right)[\![v]\!] - \frac{a_L}{v_L}\frac{v_V}{a_V} \\
&= \xi\left(1 + 2\sqrt{\frac{a_V}{v_V}\frac{a_L}{v_L}}\tilde{p}\partial_{p_L} h(\tilde{p},\varphi(\tilde{p}))\,[\![v]\!] - \frac{a_V}{v_V}\frac{v_L}{a_L}\right) \\
&\Leftrightarrow \\
&1 - \xi + \frac{a_V}{v_V}\frac{a_L}{v_L}\left(\xi\frac{v_L^2}{a_L^2} - \frac{v_V^2}{a_V^2}\right) = \dots \\
&= 2\sqrt{\frac{a_V}{v_V}\frac{a_L}{v_L}}[\![v]\!]\left(\frac{1}{\tilde{p}}\sqrt{\frac{a_V}{v_V}\frac{a_L}{v_L}} + \tilde{p}(\partial_{p_V} h(\tilde{p},\varphi(\tilde{p})) + \xi\partial_{p_L} h(\tilde{p},\varphi(\tilde{p})))\right).
\end{aligned}
\tag{3.54}
$$

For the right hand side of (3.54) we easily see

$$
2\sqrt{\frac{a_V}{v_V}\frac{a_L}{v_L}}[\![v]\!]\left(\frac{1}{\tilde{p}}\sqrt{\frac{a_V}{v_V}\frac{a_L}{v_L}} + \tilde{p}(\partial_{p_V} h + \xi\partial_{p_L} h)\right) = 2\sqrt{\frac{a_V}{v_V}\frac{a_L}{v_L}}[\![v]\!]\,z'(\tilde{p}) \geq 0.
$$

If we consider the left hand side of (3.54) as a function of ξ we get

$$
\frac{\mathrm{d}}{\mathrm{d}\xi}\left(1 - \xi + \frac{a_V}{v_V}\frac{a_L}{v_L}\left(\xi\frac{v_L^2}{a_L^2} - \frac{v_V^2}{a_V^2}\right)\right) = -1 + \frac{a_V}{a_L}\frac{v_L}{v_V} \leq -1 + \alpha\beta < 0.
$$

Thus the left hand side of (3.54) is strictly decreasing in ξ and we have

$$1-\xi+\frac{a_V}{v_V}\frac{a_L}{v_L}\left(\xi\frac{v_L^2}{a_L^2}-\frac{v_V^2}{a_V^2}\right)\overset{\xi=1}{=}\frac{a_V}{v_V}\frac{a_L}{v_L}\left[\!\!\left[\frac{v^2}{c^2}\right]\!\!\right]<0.$$

Since $\xi > 1$ the left hand side of (3.54) is negative and hence contradicts the positive right hand side. Therefore the assumption for z_{max} is wrong. □

Remark 3.3.4. *Lemma 3.3.3 is a direct improvement of Corollary 3.2.6 obtained during the proof of Theorem 3.2.2. There we stated that the upper bound a_L/v_L for the mass flux z is always fulfilled.*

Now we consider two phase flows, where we initially have the vapor phase on the left ($x < 0$) and the liquid phase on the right side ($x > 0$). The different phases are described using the corresponding *EOS*. The considered Riemann initial data is

$$\rho(x,0)=\begin{cases}\rho_V,\ x<0\\ \rho_L,\ x>0\end{cases}\quad\text{and}\quad u(x,0)=\begin{cases}u_V,\ x<0\\ u_L,\ x>0\end{cases}. \tag{3.55}$$

The solution consists of two classical waves and the phase boundary separating four constant states. Hence there are three possible wave patterns, see Figure 3.2.

3.3.1 1^{st} Case: Two Phase Flow without Phase Transition

At first we want to deal with the case where phase transition is excluded, i.e. $z = 0$. Let us consider a wave pattern of type (b), see Figure 3.2. The four constant states are denoted as follows

$$\mathbf{W}_V=\begin{pmatrix}\rho_V\\u_V\end{pmatrix},\quad \mathbf{W}_V^*=\begin{pmatrix}\rho_V^*\\u_V^*\end{pmatrix},\quad \mathbf{W}_L^*=\begin{pmatrix}\rho_L^*\\u_L^*\end{pmatrix},\quad \mathbf{W}_L=\begin{pmatrix}\rho_L\\u_L\end{pmatrix}.$$

As in 3.1.2 we want to derive a single function such that the single root p is the solution for the pressure p_V^*. This procedure again uses the constancy of pressure and velocity across the phase boundary, $u_V^* = u_L^*$ and $p_V^* = p_L^*$, which is because of $z = 0$. For the solution we use the results obtained in Section 3.1.

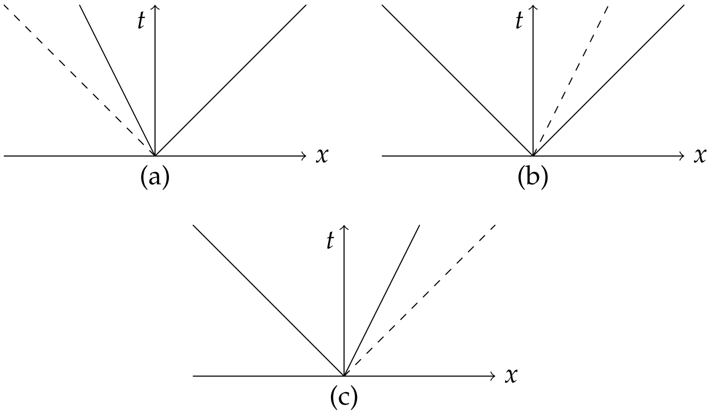

Figure 3.2: Wave patterns. Solid line: classical waves. Dashed line: phase boundary

Theorem 3.3.5 (Solution without Phase Transition)**.** *Let* $f(p, \mathbf{W}_V, \mathbf{W}_L)$ *be given as*

$$f(p, \mathbf{W}_V, \mathbf{W}_L) = f_V(p, \mathbf{W}_V) + f_L(p, \mathbf{W}_L) + \Delta u, \;\; \Delta u = u_L - u_V,$$

with the functions f_V *and* f_L *given by*

$$f_K(p, \mathbf{W}_K) = \begin{cases} \sqrt{-[\![p]\!]\,[\![v_K]\!]}, \;\; p > p_K \; \textit{(Shock)} \\ \displaystyle\int_{p_K}^{p} \frac{v_K(\zeta)}{a_K(\zeta)}\,\mathrm{d}\zeta, \;\; p \le p_K \; \textit{(Rarefaction)} \end{cases}, \quad K \in \{V, L\}.$$

If there is a root $f(p^*, \mathbf{W}_V, \mathbf{W}_L) = 0$ *with* $0 < p^* \le \tilde{p}$*, then this root is unique. Here* $\tilde{p}$ *is given as in Definition 1.4.1. Further this is the unique solution for the pressure* p_V^* *of the Riemann problem (3.1)-(3.2), (3.55). The velocity* $u^* := u_V^* = u_L^*$ *is given by*

$$u^* = \frac{1}{2}(u_L + u_V) + \frac{1}{2}(f_L(p^*, \mathbf{W}_V) - f_V(p^*, \mathbf{W}_L)).$$

Proof: The function f is strictly monotone increasing in p due to the inequalities (3.30), (3.31) and Lemma 3.3.1.
Furthermore we have $f(p, \mathbf{W}_V, \mathbf{W}_L) \to -\infty$ for $p \to 0$. Hence f has at most

one unique root, which is by construction the solution for the pressure p^*_V. The statement for the velocity u^* follows immediately from the results in Section 3.1. □

Note that one has to choose the corresponding *EOS* to calculate the pressure depending quantities according to the index $K \in \{L, V\}$.

Theorem 3.3.6 (Sufficient Condition for Solvability)**.** *Consider the Riemann problem (3.1)-(3.2), (3.55). The considered Riemann problem is solvable if and only if*

$$f(\tilde{p}, \mathbf{W}_V, \mathbf{W}_L) \geq 0.$$

Proof: As seen before in the proof of Theorem 3.3.5, f is strictly monotone increasing in p with $f(p, \mathbf{W}_V, \mathbf{W}_L) \to -\infty$ for $p \to 0$. Accordingly f has a unique root if and only if $f(p, \mathbf{W}_V, \mathbf{W}_L) \geq 0$ for $p \to \tilde{p}$. □

So far we discussed the case that the solution is of type (b). The following result deals with the cases (a) and (c).

Lemma 3.3.7. *There exists no solution of wave pattern types (a) and (c). This includes the coincidence of a classical wave and the phase boundary.*

Proof: Let us first discuss case (c). For the notation see Figure 3.3. Since $z = 0$ we have $w = u_L = u^*_V$ for the velocity of the interface. Further we assume, that the right classical wave is a shock moving with speed S. It is

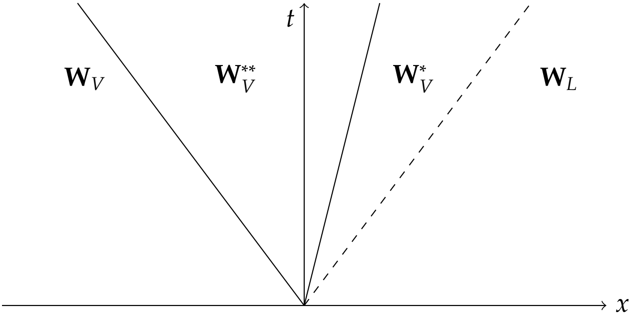

Figure 3.3: Wave pattern of type (c) with notation

obvious that $w \geq S$ must hold. For the case of a right shock we have $p_V^{**} > p_V^*$ and hence we obtain from the entropy inequality $Q > 0$, see Subsection 3.1.2. Now we make use of the continuity of the mass flux across a shock wave and obtain

$$Q = -\rho_V^*(u_V^* - S) \quad \Leftrightarrow \quad u_V^* - S = -\frac{Q}{\rho_V^*} \quad \overset{u_V^*=w}{\Leftrightarrow} \quad S = w + \frac{Q}{\rho_V^*} > w.$$

This contradicts the condition $w \geq S$. If, on the other hand, the right classical wave is a rarefaction wave we have for the head speed $u_V^* + a_V(p_V^*)$, see Subsection 3.1.2. Again this contradicts $w = u_L = u_V^* \geq u_V^* + a_V(p_V^*)$. In case that the phase boundary lies inside the rarefaction wave, we obtain similar contradictions in the wave speeds. For wave pattern type (a) the arguments are analogue. □

3.3.2 2^{nd} Case: Two Phase Flow with Phase Transition

Now we want to take phase transition into account, i.e. $z \neq 0$. As before we first want to discuss the wave pattern of type (b), see Figure 3.2. In order to determine the solution we again construct a function analogue to Subsection 3.3.1. For the left and right classical waves we use

$$u_V^* = u_V - f_V(p_V^*, \mathbf{W}_V) \quad \text{and} \quad u_L^* = u_L + f_L(p_L^*, \mathbf{W}_L). \tag{3.56}$$

Across the phase boundary we make use of the jump conditions and obtain as in Subsection 3.1.2

$$[\![u]\!] = u_L^* - u_V^* = -z\,[\![v]\!] = -z(v_L(p_L^*) - v_V(p_V^*)). \tag{3.57}$$

Finally we use the results obtained in Section 3.2, especially Theorem 3.2.2, to express the liquid pressure at the interface as a function of the interface vapor pressure $p_L = \varphi(p_V)$. Combining these considerations we end up with the following theorem.

Theorem 3.3.8 (Solution with Phase Transition). *Let $f_z(p, \mathbf{W}_V, \mathbf{W}_L)$ be given as*

$$f_z(p, \mathbf{W}_V, \mathbf{W}_L) = f_V(p, \mathbf{W}_V) + f_L(\varphi(p), \mathbf{W}_L) + z\,[\![v]\!] + \Delta u, \;\; \Delta u = u_L - u_V,$$

with the functions f_V *and* f_L *given by*

$$f_V(p,\mathbf{W}_V) = \begin{cases} \sqrt{-\,[\![p]\!]\,[\![v]\!]}, & p > p_V \ (\textit{Shock}) \\ \displaystyle\int_{p_V}^{p} \frac{v_V(\zeta)}{a_V(\zeta)}\,\mathrm{d}\zeta, & p \le p_V \ (\textit{Rarefaction}) \end{cases},$$

$$f_L(\varphi(p),\mathbf{W}_L) = \begin{cases} \sqrt{-\,[\![p]\!]\,[\![v]\!]}, & \varphi(p) > p_L \ (\textit{Shock}) \\ \displaystyle\int_{p_L}^{\varphi(p)} \frac{v_L(\zeta)}{a_L(\zeta)}\,\mathrm{d}\zeta, & \varphi(p) \le p_L \ (\textit{Rarefaction}) \end{cases}.$$

The function $\varphi(p)$ *is implicitly defined by (3.38) and the mass flux is given by (3.37). If there is a root* $f_z(p^*,\mathbf{W}_V,\mathbf{W}_L) = 0$ *with* $0 < p^* \le \tilde{p}$*, this root is unique. If further*

$$p^* > p_V \quad \textit{we must have} \quad z > -\frac{a_V(\bar{p})}{v_V(\bar{p})} \quad \textit{for} \quad \bar{p} \in (p_V, p^*). \tag{3.58}$$

Then p^* *is the unique solution for the pressure* p_V^* *of a (b)-type solution of the Riemann problem (3.1)-(3.2), (3.55) with phase transition. If there is no root or condition (3.58) is not satisfied, then there is no solution to the mentioned Riemann problem.*

Proof: Due to (3.30), (3.31), Corollary 3.2.9 and Lemma 3.3.1 we get that the function f_z is strictly monotone increasing in p. Furthermore we have $f(p,\mathbf{W}_V,\mathbf{W}_L) \to -\infty$ for $p \to 0$. Hence f has at most one unique root, which is by construction the solution for the pressure p_V^*. Theorem 3.2.2 then uniquely defines the liquid pressure $p_L^* = \varphi(p_V^*)$ and the mass flux z at the interface. The remaining quantities can be calculated using the *EOS* and (3.56). □

Remark 3.3.9. *Condition (3.58) is needed in the case of a shock wave in the (left) vapor phase to guarantee that* $w > S$*. Where* w *denotes the velocity of the interface and* S *of the shock respectively. This can be obtained as follows*

$$u_V^* - S = -v_V(p_V^*)Q_S \quad \textit{and} \quad u_V^* - w = -v_V(p_V^*)z \quad \Leftrightarrow \quad w - S = v_V(p_V^*)(z - Q_S)$$
$$\Rightarrow \quad w > S \quad \Leftrightarrow \quad z > Q_S = -\frac{a_V(\bar{p})}{v_V(\bar{p})}.$$

For the last equality we used the Lax condition for S together with the monotonicity of $a(p)/v(p)$. If this condition is not satisfied by the root $f_z(p^*, \mathbf{W}_V, \mathbf{W}_L) = 0$, the root is meaningless.

Theorem 3.3.10 (Sufficient Condition for Solvability I)**.** *If the Riemann problem (3.1)-(3.2), (3.55) is solvable without phase transition, see Subsection 3.3.1, then the same Riemann problem is also solvable taking into account phase transition according to the kinetic relation (3.37).*

Proof:
First Case $f(p^*, \mathbf{W}_V, \mathbf{W}_L) = 0$ with $p^* = p_0$: In view of Section 3.2 we have $p_0 = \varphi(p^*)$, $z = 0$ and hence $f_z(p^*, \mathbf{W}_V, \mathbf{W}_L) = 0$.

Second Case $f(p^*, \mathbf{W}_V, \mathbf{W}_L) = 0$ with $p^* > p_0$: From that we have

$$\varphi(p^*) \overset{3.2.2}{>} p^* > p_0 \quad \text{and} \quad z(p^*) = p^* h(p^*, \varphi(p^*)) < 0.$$

This gives

$$f_z(p^*, \mathbf{W}_V, \mathbf{W}_L) > f(p^*, \mathbf{W}_V, \mathbf{W}_L) = 0.$$

So there exists a $p_V^* < p^*$ such that $f_z(p_V^*, \mathbf{W}_V, \mathbf{W}_L) = 0$.

Third Case $f(p^*, \mathbf{W}_V, \mathbf{W}_L) = 0$ with $p^* < p_0$: In this situation we obtain

$$0 = f(p^*, \mathbf{W}_V, \mathbf{W}_L) \overset{p^*<p_0}{<} f(p_0, \mathbf{W}_V, \mathbf{W}_L) \overset{\varphi(p_0)=p_0, z=0}{=} f_z(p_0, \mathbf{W}_V, \mathbf{W}_L)$$

Hence there exists a $p_V^* < p_0$ such that $f_z(p_V^*, \mathbf{W}_V, \mathbf{W}_L) = 0$. □

Corollary 3.3.11. *Consider the Riemann problem (3.1)-(3.2), (3.55) without phase transition and let p^* be the solution for the pressure. Then we have for the same Riemann problem with phase transition and the corresponding solutions p_V^* and $p_L^* = \varphi(p_V^*)$ the following relations:*

(1) $p^* = p_0$ implies $p_V^* = p_L^* = p_0$, i.e. equilibrium.

(2) $p^* > p_0$ implies $p_0 < p_V^* < p^*$, i.e. condensation.

(3) $p^* < p_0$ implies $p^* < p_L^* < p_0$, i.e. evaporation.

Proof: The equilibrium case is obvious. The inequality $p_V^* < p^*$ in the second was obtained in the second part in the proof of Theorem 3.3.10. It remains to show that $p_0 < p_V^*$. Assume that $p_V^* \le p_0$, this gives

$$\begin{aligned} 0 &= f_z(p_V^*, \mathbf{W}_V, \mathbf{W}_L) \le f_z(p_0, \mathbf{W}_V, \mathbf{W}_L) \\ &= f(p_0, \mathbf{W}_V, \mathbf{W}_L) \overset{p_0<p^*}{<} f(p^*, \mathbf{W}_V, \mathbf{W}_L) = 0. \end{aligned}$$

For the evaporation case the inequality $p_L^* < p_0$ is a consequence of the third part in the proof of Theorem 3.3.10. There we obtained $p_V^* < p_0$ and this gives, together with Theorem 3.2.2, the second inequality. Finally we want to prove the first inequality $p^* < p_L^*$. Again using Theorem 3.2.2 gives $p_V^* > p_0$ if we assume $p_L^* > p_0$. By an analogous argument as for the second case this leads to a contradiction. Thus we have $p_L^* < p_0$. □

Theorem 3.3.12 (Sufficient Condition for Solvability II)**.** *Consider the Riemann problem (3.1)-(3.2), (3.55) with phase transition. This Riemann problem is solvable by a (b)-type solution if and only if condition (3.58) holds and*

$$f_z(\tilde{p}, \mathbf{W}_V, \mathbf{W}_L) \ge 0.$$

Proof: The statement is obvious, since it guarantees a root for f_z. □

As in Subsection 3.3.1 we want to discuss wave patterns of type (a) and (c) for the Riemann problem (3.1)-(3.2), (3.55) with phase transition. The results are given in the subsequent three lemmata.

Lemma 3.3.13. *There is no solution with a wave pattern of type (a).*

Proof: Assume there is a solution of type (a) as in Figure 3.4. In this case we observe condensation and according to Corollary 3.2.10 we have

$$z < 0 \quad \text{and} \quad p_0 < p_V < p_L^*.$$

Let us first assume that the left classical wave is a rarefaction wave. The head speed is given by $S = u_L^* - a_L(p_L^*)$ and we obtain

$$w = v_L(p_L^*)z + u_L^* \overset{(a)}{\le} S = u_L^* - a_L(p_L^*) \quad \Leftrightarrow \quad z \le -\frac{a_L(p_L^*)}{v_L(p_L^*)} \overset{(3.52)}{<} -\frac{a_V}{v_V}$$

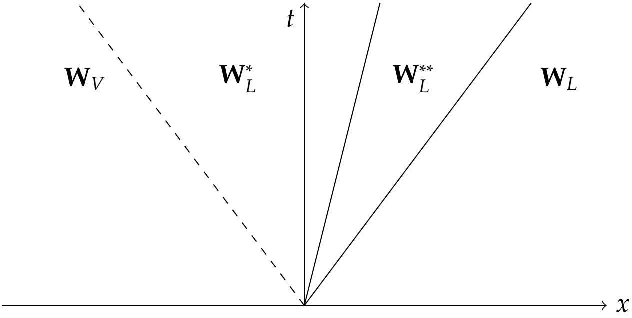

Figure 3.4: Wave pattern of type (a) with notation

This is a contradiction and thus we can exclude this case. Given a shock instead of a rarefaction wave we have using (3.23) and the Lax condition

$$u_L^* - a_L(p_L^*) > S = u_L^* + v_L(p_L^*)Q_S > u_L^{**} - a_L(p_L^{**}) \text{ with } Q_S = -\frac{a_L(\bar{p}_L)}{v_L(\bar{p}_L)},\ \bar{p}_L \in (p_L^*, p_L^{**}).$$

Hence we yield

$$w < S \quad \Leftrightarrow \quad z < Q_S = -\frac{a_L(\bar{p}_L)}{v_L(\bar{p}_L)} \overset{p_L^* < \bar{p}_L}{<} -\frac{a_L(p_L^*)}{v_L(p_L^*)} \overset{(3.52)}{<} -\frac{a_V}{v_V}.$$

Therefore we can also exclude this case with respect to condition (3.58) and the proof is finished. □

Lemma 3.3.14. *For the considered Riemann problem with phase transition exists no solution of type (c) with* $p_L \geq p_0$.

Proof: A solution of type (c) implies an evaporation process which requires $p_L < p_0$. □

Lemma 3.3.15. *For* $p_L \in (\hat{p}_L, p_0]$ *exists no solution of type (c) of the considered Riemann problem with phase transition.*

Proof: Assume we have a wave pattern of type (c) as in Figure 3.3. Hence we have evaporation and according to Corollary 3.2.10 we have

$$z > 0 \quad \text{and} \quad p_V^* < p_L < p_0.$$

Let us first assume that the right classical wave is a rarefaction wave. The head speed is given by $S = u_V^* + a_V(p_V^*)$ and we obtain

$$w = v_V(p_V^*)z + u_V^* \overset{(c)}{\geq} S = u_V^* + a_V(p_V^*) \quad \Leftrightarrow \quad z \geq \frac{a_V(p_V^*)}{v_V(p_V^*)}.$$

For a right shock ($Q_S > 0$) we have using (3.23) and the Lax condition

$$\begin{aligned} & u_V^{**} + a_V(p_V^{**}) > S = u_V^* + v_V(p_V^*)Q_S > u_V^* + a_V(p_V^*) \\ & \text{with} \quad Q_S = \frac{a_V(\bar{p}_V)}{v_V(\bar{p}_V)}, \quad \bar{p}_V \in (p_V^*, p_V^{**}). \end{aligned}$$

Hence we yield

$$w > S \quad \Leftrightarrow \quad z > Q_S = \frac{a_V(\bar{p}_V)}{v_V(\bar{p}_V)} \overset{\bar{p}_V > p_V^*}{>} \frac{a_V(p_V^*)}{v_V(p_V^*)}.$$

Due to Lemma 3.3.3 we have an upper bound for the mass flux that does not initially exclude the conditions derived above for the rarefaction and shock wave. But the two cases are excluded if $z < a_V(p_V^*)/v_V(p_V^*)$. Indeed we have due to the monotonicity of z and a/v that

$$\exists\ \hat{p}_V < p_0 \quad \text{such that} \quad \forall p_V \in (\hat{p}_V, p_0] : z(p_V) < \frac{a_V(p_V)}{v_V(p_V)}.$$

Due to the strict monotonicity of $p_L = \varphi(p_V^*)$, see Theorem 3.2.2, the proof is complete. □

3.4 Phase Creation in Single Phase Flows

3.4.1 Condensation by Compression

Let us consider the following Riemann initial data with $\rho_{V^\pm} \in (0, \tilde{\rho}]$

$$\rho(x,0) = \begin{cases} \rho_{V^-},\ x < 0 \\ \rho_{V^+},\ x > 0 \end{cases} \quad \text{and} \quad u(x,0) = \begin{cases} u_{V^-},\ x < 0 \\ u_{V^+},\ x > 0 \end{cases}. \tag{3.59}$$

Hence initially we have a Riemann problem for a single vapor phase and therefore we can directly apply the results obtained in Subsection 3.1.2.

Theorem 3.4.1 (Solution of Isothermal Euler Equations for a Single Vapor Phase)**.** *Let* $f(p, \mathbf{W}_{V^-}, \mathbf{W}_{V^+})$ *be given as*

$$f(p, \mathbf{W}_{V^-}, \mathbf{W}_{V^+}) = f_-(p, \mathbf{W}_{V^-}) + f_+(p, \mathbf{W}_{V^+}) + \Delta u, \ \Delta u = u_{V^+} - u_{V^-},$$

with the functions f_- *and* f_+ *given by*

$$f_\pm(p, \mathbf{W}_{V^\pm}) = \begin{cases} \sqrt{-[\![p]\!]\,[\![v]\!]}, & p > p_{V^\pm} \text{ (Shock)} \\ \displaystyle\int_{p_{V^\pm}}^{p} \frac{v_V(\zeta)}{a_V(\zeta)}\,\mathrm{d}\zeta, & p \le p_{V^\pm} \text{ (Rarefaction)} \end{cases}.$$

If there is a root $f(p^*, \mathbf{W}_{V^-}, \mathbf{W}_{V^+}) = 0$ *with* $0 < p^* \le \tilde{p}$*, then this root is unique. Further this is the unique solution for the pressure* p_V^* *of the Riemann problem (3.1) - (3.2), (3.59). The velocity* u_V^* *is given by*

$$u_V^* = \frac{1}{2}(u_{V^+} + u_{V^-}) + \frac{1}{2}(f_+(p^*, \mathbf{W}_{V^+}) - f_-(p^*, \mathbf{W}_{V^-})).$$

This is no new result and therefore it is well known, cf. Toro [78]. Usually one looks for a pressure p^* that solves $f(p, \mathbf{W}_{V^-}, \mathbf{W}_{V^+}) = 0$. Due to the asymptotic behavior there is always a solution. Nevertheless a solution with an unreasonable large vapor pressure is physically not meaningful, since a sufficiently high pressure in a gas will lead to a phase transition to a liquid or even solid phase. According to [37] we also only consider solutions which satisfy $0 < p^* \le \tilde{p}$, where $\tilde{p}$ again denotes the maximal gas pressure. This being said, we can find Riemann initial data without a solution. In this case proceed as follows.

Definition 3.4.2 (Nucleation Criterion)**.** *If there is no solution of the Riemann problem (3.1) - (3.2), (3.59) according to Theorem 3.4.1, then nucleation occurs.*

If this criterion is fulfilled, we search a solution consisting of two classical waves and two phase boundaries. In the following we will again discuss several wave patterns.

Lemma 3.4.3. *If there is a solution of the Riemann problem (3.1) - (3.2), (3.59) with two classical waves and two phase boundaries, then no wave is propagating inside the liquid phase. Hence classical waves may only occur in the vapor phase.*

Proof: Assume a left going classical wave is propagating through the liquid phase. We denote the liquid states left and right to this wave by $\mathbf{W}_L^*$

and $\mathbf{W}_L^{**}$. Further left to this classical wave there is a phase boundary moving with speed w_1. The vapor state left to this phase boundary is denoted by $\mathbf{W}_V^*$. Obviously this must be a condensation process and accordingly $p^* > p_0$ and $p_L^* > p_0$. This configuration is excluded by Lemma 3.3.13. Analogously we can discuss the case of a right going classical wave. □

As a consequence of the above result classical waves only propagate through the vapor phase. Hence we further have to discuss the following three patterns, see Figure 3.5.

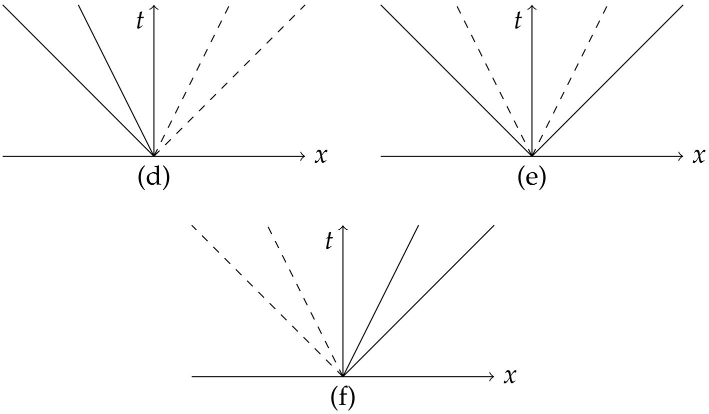

Figure 3.5: Wave patterns. Solid line: classical wave. Dashed line: phase boundary

Lemma 3.4.4. *There are no solutions of wave pattern types (d) and (f).*

Proof: A solution with type (d) wave pattern corresponds to wave pattern type (c) in the previous Subsection 3.3.2, see Figure 3.3. Thus by Lemma 3.3.14 and Lemma 3.3.15 we know that this is only possible for sufficiently small pressures and therefore implies evaporation. Since we have a condensation process wave pattern type (d) can be excluded. Analogously we discuss a type (f) solution. This corresponds to a type (a) solution in Subsection 3.3.2, see Figure 3.4. Hence due to Lemma 3.3.13 a solution of wave pattern type (f) is also impossible. □

Consequently the only possible wave pattern in this case is of type (e), see Figure 3.6.

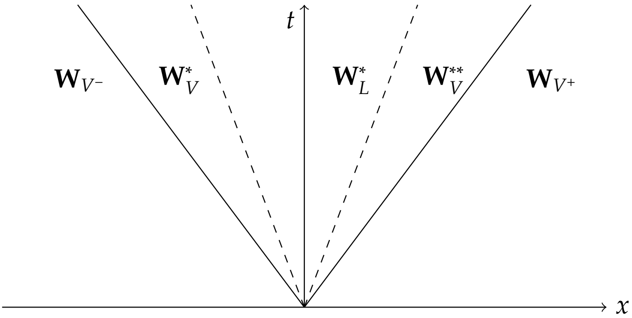

Figure 3.6: Wave pattern of type (e) with notation

Lemma 3.4.5. *For a solution of wave pattern type (e) the equality* $p_V^* = p_V^{**}$ *holds.*

Proof: Across the left phase boundary the liquid pressure p_L^* is uniquely defined by the vapor pressure p_V^* using Theorem 3.2.2. So far we assumed the vapor left of the liquid phase. For the right phase boundary the opposite is the case and thus we have to use the kinetic relation (3.35). Nevertheless the results of the previous section remain unchanged and hence we obtain the same function to determine the liquid pressure

$$p_L^* = \varphi(p_V^*) = \varphi(p_V^{**}).$$

Hence the vapor pressures are equal. □

Taking into account that there are two phase boundaries and using the results obtained in the previous sections we can state the following theorem.

Theorem 3.4.6 (Solution of Isothermal Euler Equations for Two Vapor States with Phase Transition)**.** *Consider the Riemann problem (3.1) - (3.2), (3.59) and assume the nucleation criterion is satisfied. Let* $f_z(p, \mathbf{W}_{V^-}, \mathbf{W}_{V^+})$ *be given as*

$$f_z(p, \mathbf{W}_{V^-}, \mathbf{W}_{V^+}) = f_-(p, \mathbf{W}_{V^-}) + f_+(p, \mathbf{W}_{V^+}) + 2z [\![v]\!] + \Delta u, \;\; \Delta u = u_{V^+} - u_{V^-},$$

with the functions f_- *and* f_+ *given by*

$$f_\pm(p, \mathbf{W}_{V^\pm}) = \begin{cases} \sqrt{-[\![p]\!]\,[\![v]\!]}, & p > p_{V^\pm} \text{ (Shock)} \\ \displaystyle\int_{p_{V^\pm}}^{p} \frac{v_V(\zeta)}{a_V(\zeta)}\, \mathrm{d}\zeta, & p \le p_{V^\pm} \text{ (Rarefaction)} \end{cases}.$$

Here z *is given by (3.34) and* $[\![v]\!] = v_L(\varphi(p)) - v_V(p)$*. The function* φ *is implicitly defined by (3.38). If there is a root* $f_z(p^*, \mathbf{W}_{V^-}, \mathbf{W}_{V^+}) = 0$ *with* $p_0 < p^* \le \tilde{p}$*, then this root is the only one. Further this is the unique solution for the vapor pressures* $p_V^* = p_V^{**}$ *of the Riemann problem (3.1) - (3.2), (3.59). The liquid velocity* u_L^* *is given by*

$$u_L^* = \frac{1}{2}(u_{V^+} + u_{V^-}) + \frac{1}{2}(f_+(p^*, \mathbf{W}_{V^+}) - f_-(p^*, \mathbf{W}_{V^-})).$$

By the previous results it is obvious that f_z has at most one root. By construction this root is the solution for the vapor pressure in the two star regions, see Figure 3.6. The following results are completely analogue to those obtained before for the two phase case.

Remark 3.4.7. *Note that* $u_V^* \neq u_V^{**}$ *with* $u_V^* + u_V^{**} = 2u_L^*$*.*

Theorem 3.4.8 (Sufficient Condition for Solvability I)**.** *Consider the Riemann problem (3.1) - (3.2), (3.59). This problem is solvable without phase transition if and only if*

$$f(\tilde{p}, \mathbf{W}_{V^-}, \mathbf{W}_{V^+}) \ge 0.$$

Here f *is given as in Theorem 3.4.1.*

Proof: This statement is obvious due to the monotonicity of f. □

Theorem 3.4.9 (Sufficient Condition for Solvability II)**.** *Consider the Riemann problem (3.1) - (3.2), (3.59) and assume the nucleation criterion is satisfied. Accounting for phase transition, this problem is solvable if and only if*

$$f_z(\tilde{p}, \mathbf{W}_{V^-}, \mathbf{W}_{V^+}) \ge 0.$$

The function f_z *is defined as in Theorem 3.4.6.*

Proof: Again the statement is obvious due to the monotonicity of f_z. □

3.4.2 Evaporation by Expansion

Now we consider the following Riemann initial data with $\rho_{L^\pm} \geq \rho_L^{min}$

$$\rho(x,0) = \begin{cases} \rho_{L^-}, & x < 0 \\ \rho_{L^+}, & x > 0 \end{cases} \quad \text{and} \quad u(x,0) = \begin{cases} u_{L^-}, & x < 0 \\ u_{L^+}, & x > 0 \end{cases}. \tag{3.60}$$

Hence initially we have a Riemann problem for a single liquid phase. We have seen so far that at a planar phase boundary the liquid pressure is always positive. However it is known that negative liquid pressures are possible, cf. Davitt et al. [19] for water. This gives rise to cavitation in the liquid phase. Again, in the liquid-vapor case a negative liquid pressure is forbidden, see (3.41). Nevertheless in the liquid-liquid case we may encounter negative liquid pressures. We define the smallest possible liquid pressure to be p_{min} and with this definition we obtain the following result.

Theorem 3.4.10 (Solution of Isothermal Euler Equations for a Single Liquid Phase)**.** *Let* $f(p, \mathbf{W}_{L^-}, \mathbf{W}_{L^+})$ *be given as*

$$f(p, \mathbf{W}_{L^-}, \mathbf{W}_{L^+}) = f_-(p, \mathbf{W}_{L^-}) + f_+(p, \mathbf{W}_{L^+}) + \Delta u, \;\; \Delta u = u_{L^+} - u_{L^-},$$

with the functions f_- *and* f_+ *given by*

$$f_\pm(p, \mathbf{W}_{L^\pm}) = \begin{cases} \sqrt{-[\![p]\!]\,[\![v]\!]}, & p > p_{L^\pm} \text{ (Shock)} \\ \displaystyle\int_{p_{L^\pm}}^{p} \frac{v_L(\zeta)}{a_L(\zeta)}\,\mathrm{d}\zeta, & p \leq p_{L^\pm} \text{ (Rarefaction)} \end{cases}.$$

If there is a root $f(p^*, \mathbf{W}_{L^-}, \mathbf{W}_{L^+}) = 0$ *with* $p_{min} \leq p^*$*, then this root is unique. Further this is the unique solution for the pressure* p_L^* *of the Riemann problem (3.1) - (3.2), (3.60). The velocity* u_L^* *is given by*

$$u_L^* = \frac{1}{2}(u_{L^+} + u_{L^-}) + \frac{1}{2}(f_+(p^*, \mathbf{W}_{L^+}) - f_-(p^*, \mathbf{W}_{L^-})).$$

Remark 3.4.11. *For simplicity we choose* $p_{min} = 0$ *but lower values are possible and the theoretical results do not depend on the specific value of* p_{min}*.*

Analogously to the case of nucleation we define the following.

Definition 3.4.12 (Cavitation Criterion)**.** *If there is no solution of the Riemann problem (3.1) - (3.2), (3.60) according to Theorem 3.4.10, then cavitation may occur.*

If this criterion is fulfilled, we look for a solution involving a vapor phase, two phase boundaries and two classical waves. Again we discuss the possible patterns.

Lemma 3.4.13. *Assume there is a solution of the Riemann problem (3.1) - (3.2), (3.60) consisting of two classical waves and two phase boundaries. If the pressures* p_{L^-}, p_{L^+} *are sufficiently large then no wave travels through the vapor.*

The proof is analogue to the one of Lemma 3.3.15.

Lemma 3.4.14. *There is no solution of type (d) or (f); see Figure 3.5.*

The proof of this lemma is analogue to the one of Lemma 3.4.4. Accordingly we construct solutions of type (e), see Figure 3.7.

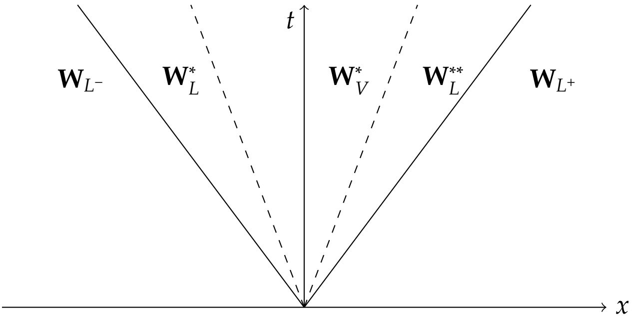

Figure 3.7: Wave pattern of type (e) with notation for the liquid case

Theorem 3.4.15 (Solution of Isothermal Euler Equations for Two Liquid States with Phase Transition)**.** *Consider the Riemann problem (3.1) - (3.2), (3.60) and assume the cavitation criterion is satisfied. Let* $f_z(p, \mathbf{W}_{L^-}, \mathbf{W}_{L^+})$ *be given as*

$$f_z(p, \mathbf{W}_{L^-}, \mathbf{W}_{L^+}) = f_-(p, \mathbf{W}_{L^-}) + f_+(p, \mathbf{W}_{L^+}) + 2z\,[\![v]\!] + \Delta u, \;\; \Delta u = u_{L^+} - u_{L^-},$$

with the functions f_- *and* f_+ *given by*

$$f_\pm(p, \mathbf{W}_{L^\pm}) = \begin{cases} \sqrt{-[\![p]\!]\,[\![v]\!]}, & \varphi(p) > p_{L^\pm} \text{ (Shock)} \\ \displaystyle\int_{p_{L^\pm}}^{\varphi(p)} \frac{v_L(\zeta)}{a_L(\zeta)}\,\mathrm{d}\zeta, & \varphi(p) \le p_{L^\pm} \text{ (Rarefaction)} \end{cases}.$$

Here z is given by (3.34) and $[\![v]\!] = v_L(\varphi(p)) - v_V(p)$. The function φ is implicitly defined by (3.38). If there is a root $f_z(p^*, \mathbf{W}_{L^-}, \mathbf{W}_{L^+}) = 0$ with $p_{min} \leq p^*$, then this root is unique. Further this is the unique solution for the vapor pressures p_V^* of the Riemann problem (3.1) - (3.2), (3.60). The vapor velocity u_V^* is given by

$$u_V^* = \frac{1}{2}(u_{L^+} + u_{L^-}) + \frac{1}{2}(f_+(p^*, \mathbf{W}_{L^+}) - f_-(p^*, \mathbf{W}_{L^-})).$$

Proof: Due to the previous results, the function f_z has at most one root. This root is by construction the solution for the vapor pressure in the star region. □

Completely analogue to the condensation case, see Subsection 3.4.1, we have the following results.

Theorem 3.4.16 (Sufficient Condition for Solvability I)**.** *Consider the Riemann problem (3.1) - (3.2), (3.60). This problem is solvable without phase transition if and only if*

$$f(p_{min}, \mathbf{W}_{L^-}, \mathbf{W}_{L^+}) \leq 0.$$

Here f is given as in Theorem 3.4.10.

Proof: The statement is easily verified due to the monotonicity of f. □

Theorem 3.4.17 (Sufficient Condition for Solvability II)**.** *Consider the Riemann problem (3.1) - (3.2), (3.60) and assume the cavitation criterion is satisfied. If we admit phase transition, this problem is always solvable.*

Proof: This statement is obvious due to the fact that $z\,[\![v]\!] \to -\infty$ for $p_V^* \to 0$. □

3.5 Conclusion

3.5.1 Discussion of the Assumptions

In this part we now want to discuss the assumptions previously made to solve the problem. Basically we have three types of requirements. First there are the ones due to the underlying thermodynamics, in particular the first and second law of thermodynamics. Second there are conditions, one needs to solve the single phase Riemann problem for the Euler equations. The third type concerns the assumptions imposed to solve the two phase problem. Note that the assumptions are sufficient, from a mathematical point of view, to obtain the results presented throughout this work.

From a thermodynamic point of view we have first and foremost to satisfy the first and second law of thermodynamics including the requirement of thermodynamic stability (3.7). This is obtained by deriving the pressure law from a suited thermodynamic potential.
The conditions imposed on the EOS in order to solve the (single phase) Riemann problem for the Euler equations are

$$\gamma > 0, \quad \mathcal{G} > 0, \quad v(p) \overset{p\to\infty}{\to} 0, \quad \text{and} \quad v(p) \overset{p\to 0}{\to} \infty$$

That we require the single phase Riemann problem to be solvable is of course reasonable, since otherwise any further discussion would be unnecessary. The conditions above are completely analogue to those stated in [60]. Note that for any EOS where the speed of sound is a constant (such as in [37]) we have $\mathcal{G} = 1$. We want to point out that the aforementioned requirements of type one and two are basically no new or additional assumptions since they are already needed to treat the single phase case.

Since we are concerned with discussing the case of two phases it is reasonable to assume that all single phase requirements are met and only a few new ones need to be added. In order to solve the two phase Riemann problem we need the additional assumptions (3.39) and (3.52).
The uniform upper bound for the quotient of the specific volumes basically tells us how close we can get to the critical point, where the volumes would become equal. The case of $\alpha = 1$, i.e. we include the critical point where the volumes become equal, is not considered here and has to be treated separately.
The constant β bounds the quotient of the sound speeds and is only needed to be strict smaller than $1/\alpha$.
The assumption on the lower bound of γ_V in (3.39) is a rather technical one. Nevertheless if we assume τ to be as in (3.36) and consider the ideal gas EOS for the vapor phase we have

$$1 = \gamma_V > \tau a_V^3 (1-\alpha)^2 = \frac{1}{\sqrt{2\pi}} \left(\frac{m}{kT_0}\right)^{\frac{3}{2}} (1-\alpha)^2 a_V^3 = \frac{(1-\alpha)^2}{\sqrt{2\pi}}.$$

Hence this bound is easily satisfied. If the sound speed of the vapor phase would depend on the pressure one would have to check this requirement more carefully. We further want to emphasize that apart from $\tau > 0$ and $(3.39)_3$ we do not assume any particular shape or even magnitude of τ. This is a further key point that contributes to the generality of our result.
The last requirement in (3.39) is concerned with the maximum vapor pressure. Due to this bound the vapor is allowed to be compressed (depending on α) with more than the saturation pressure. This allows metastable states, which is reflected in the Maxwell construction. Here of course one has to make sure that the maximum vapor pressure $\tilde{p}$ defined in Definition 1.4.1 satisfies this bound. This can be guaranteed by choosing an appropriate temperature and also how the two EOS are connected by $\bar{v}(p)$ in Definition 1.4.1. Usually $\tilde{p}$ will only be slightly larger than the saturation pressure for a wide range of temperatures.

Now we want to comment assumptions (3.52). Let us first consider γ_L. Over wide temperature ranges we have $\gamma_L \geq 1$ for many substances. For example in Subsection 3.5.2 we consider the *linear* and *nonlinear Tait* EOS for liquid water and for this type of EOS modeling water this is true up to 636.165 K. A similar result can be obtained for the *van der Waals* EOS. Above that temperature it is not possible to use the ideal (polytropic) gas EOS together with such a liquid EOS, because it would contradict (3.52) (**II**). Regarding case (**II**) we want to emphasize that for $1 > \gamma_L > \gamma_V$ the inequality including α is trivial. In fact in numerical studies we exemplary obtained that this property is also true for the van der Waals EOS up to $\approx 640\,\mathrm{K}$.
Now we want to comment on $\varepsilon(\gamma_V)$ in (3.53). Using the ideal gas or the polytropic gas EOS gives $\gamma_V = 1$ and hence

$$\varepsilon_0 := \varepsilon(1) = -\tau a_V^3 (1-\alpha)^2 \left(1 - (\alpha\beta)^2\right) < 0.$$

We consider (3.52) (**II**) and have $1 + \varepsilon_0/\alpha < 0$ over large temperature ranges. Suppose this term becomes positive at high temperatures, it is however still smaller than one. Whereas at the same time γ_L approaches one. Hence this bound may be still valid. This of course has to be checked for any given EOS.

3.5.2 Examples

Now we want to present several examples of choices for the equations of state used to model the fluid under consideration, in this case water. First we will discuss the ideal gas EOS for the vapor phase and the (linear) Tait EOS for the liquid phase as in [37]. For the ideal gas we obtain as in Proposition 1.3.9

$$p_V(v_V) = \frac{kT_0}{m_W}\frac{1}{v_V}, \quad \gamma_V = 1, \quad \mathcal{G}_V = 1. \tag{3.61}$$

Here k is the Boltzmann constant, T_0 is the fixed temperature and m_W denotes the mass of a single water molecule. Considering the liquid phase we obtain as in Proposition 1.3.11

$$p_L(v_L) = p_0 + K_0\left(\frac{v_0}{v_L} - 1\right), \quad \gamma_L = \left(1 + \frac{v_L}{K_0 v_0}(p_0 - K_0)\right)^{-1} \overset{K_0 \geq p_0}{\geq} 1, \quad \mathcal{G}_L = 1. \tag{3.62}$$

The quantities with index zero are calculated at the saturation state corresponding to T_0. We further have the saturation pressure p_0, the modulus of compression K_0 and the specific liquid volume v_0, cf. [84]. Note that the relation $K_0 \geq p_0$ breaks down for temperatures *above* 636.165 K ($T_c = 647.096$ K). Both EOS are linear functions of the mass density and thus it is reasonable to connect them with a linear function $\bar{p}$. Hence we obtain the specific volume of the vapor phase corresponding to the maximum vapor pressure $\tilde{p}$ according to Definition 1.4.1 as the solution of the following equation

$$0 = K_0 v_0 \ln\frac{v_0}{v_m} + \frac{\tilde{v}}{v_m} - \tilde{v}\frac{kT_0}{m_W}\ln\frac{\tilde{v}}{v_m} + \frac{kT_0}{m_W}\ln\frac{v_V(p_0)}{v_m}. \tag{3.63}$$

Here v_m is chosen such that

$$v_m = \begin{cases} v_0\left(1 - \dfrac{p_0}{K_0}\right)^{-1}, T_0 \leq 620\,\text{K}, \\ v_0\left(1 + \dfrac{T_c - T_0}{T_c}\right), T_0 > 620\,\text{K}. \end{cases}$$

Using (3.63) we can calculate the quotient $v_m/\tilde{v}$ for every reasonable temperature and thus obtain α and also β. Now we can check the assumptions given in (3.39), (3.52). We have for temperatures up to 636.165 K the following

$$\alpha \lesssim 0.1949, \quad \alpha\beta \lesssim 0.5419, \quad \frac{1}{\gamma_L} - \left(1 + \frac{\varepsilon_0}{\alpha}\right) \gtrsim 0.7484 \quad \text{and} \quad \tilde{p} \lesssim 1.4825 p_0.$$

Thus all requirements are met as expected and the limiting factor here are not the assumptions but the choice of the EOS.

Remark 3.5.1. *Note that in the isothermal case the linear Tait EOS is equivalent to the stiffend gas EOS*

$$p_L(v_L) = C(\gamma-1)\frac{T_0}{v_L} - p_c \quad \textit{with} \quad C(\gamma-1) = \frac{K_0 v_0}{T_0} \quad \textit{and} \quad p_c = K_0 - p_0.$$

As a second example we want to use the nonlinear Tait EOS instead of the linear one, i.e.

$$p_L(v_L) = p_0 + K_0\left(\left(\frac{v_0}{v_L}\right)^{\nu} - 1\right), \ \nu > 1. \tag{3.64}$$

Again we use the ideal gas EOS for the vapor phase. We obtain for the nonlinear Tait EOS as in Proposition 1.3.11

$$\gamma_L = \nu\left(1 + \left(\frac{v_L}{v_0}\right)^{\nu}\left(\frac{p_0}{K_0} - 1\right)\right)^{-1} > 1, \quad \mathcal{G}_L = \frac{\nu+1}{2}$$

and

$$v_m = \begin{cases} v_0\left(1 - \dfrac{p_0}{K_0}\right)^{-\frac{1}{\nu}}, T_0 \leq 620\,\mathrm{K}, \\ v_0\left(1 + \dfrac{T_c - T_0}{T_c}\right), T_0 > 620\,\mathrm{K}. \end{cases}$$

Next with an approach analogue to the previous case we obtain $\tilde{v}$ as solution of the following equation and then calculate $\tilde{p}$

$$\begin{aligned} 0 = (p_0 - K_0)v_m + K_0 v_0 + \frac{K_0 v_0^{\nu}}{1-\nu}\left(\frac{1}{v_m^{\nu-1}} - \frac{1}{v_0^{\nu-1}}\right) \\ + \frac{v_m}{v_m - \tilde{v}}\frac{kT_0}{m_W}\ln\frac{\tilde{v}}{v_m} + \frac{kT_0}{m_W}\ln\frac{v_V(p_0)}{\tilde{v}}. \end{aligned} \tag{3.65}$$

We can use (3.65) to calculate the quotient $v_m/\tilde{v}$ for every reasonable temperature and thus obtain α and also β. Here we use $\nu = 7$ as in [72]. We again check the assumptions given in (3.39), (3.52) and obtain for temperatures up to 636.165 K the following

$$\alpha \lesssim 0.1645, \quad \alpha\beta \lesssim 0.1818, \quad \frac{1}{\gamma_L} - \left(1 + \frac{\varepsilon_0}{\alpha}\right) \gtrsim 0.7795 \quad \text{and} \quad \tilde{p} \lesssim 1.2511 p_0.$$

Hence this choice of EOS is also suitable for solving this problem for temperatures from 273.15 K up to 636.165 K. Again the limiting factor here are not the assumptions but the choice of the EOS.

3.5.3 Conclusion

The aim of the present work was to investigate the Riemann problem for the isothermal Euler equations when liquid and vapor phases are present which may condensate or evaporate. We proved that there exist unique solutions under the given assumptions.To this end we allow any EOS which satisfies these assumptions, especially nonlinear ones. This is a huge improvement to the previous work [37] where only two specific linear EOS were chosen to solve this problem. In contrast to this we for example allow the speed of sound to depend on the pressure or volume instead of being constant. Concerning [30] a key difference is that they focus on the *van-der-Waals* EOS. Further they proof uniqueness in the case when $\mathcal{G} < 0$ in the vapor phase. Physically this implies that the vapor state lies in the metastable region of the phase space. Furthermore we allow phase transitions where the pressures are not in equilibrium as for example in [24]. Additionally we can treat nucleation an cavitation. In view of the work by Hantke, T. [39] the last point has to be emphasized. To our knowledge this is the most general result concerning Riemann problems for isothermal two phase flows.

4

Isothermal Case: Numerical Solution of the Riemann Problem

Introduction

In this chapter we want to present a numerical procedure for solving the two phase flow problems presented in the previous Chapter 3. Thus we rely on the framework introduced in Section 3.1 and the results obtained in the subsequent Sections 3.2, 3.3 and 3.4. Just to give a brief summary, we considered two phase flow problems including nucleation and cavitation. The interface between the adjacent phases is given by a sharp interface and the mass transfer is controlled using the kinetic relation (3.34). For the principle aspects of the numerical treatment of hyperbolic conservation laws we recommend the books of Kröner [50], LeVeque [56] and Toro [78] and the references therein. Here our main focus is on the discussion of the vapor/liquid interface. Since there the main difficulties will arise. Once we solved this case, we can also deal with the cases of nucleation and cavitation. This chapter is organized in the following way. First we summarize the problem and point out the main challenges in Section 4.1. The numerical method, with focus on the phase boundary, is introduced in Section 4.2. It is most desirable to obtain a direct solver to omit costly iterations. Therefore we suggest in Section 4.3 a direct calculation of the liquid pressure, in terms of the vapor pressure, at the interface. In Section 4.4 we discuss the numerical procedure in the case of cavitation and nucleation. We close this chapter with the numerical test cases given in Section 4.5.

4.1 Problem Formulation and Main Challenges

Let us briefly summarize the problem we want to solve. As in Chapter 3 we study inviscid, compressible and isothermal two phase flows. The two phases are either the liquid or the vapor phase of one substance. The phases are distinguished by the *mass density* ρ and further described by the *velocity* u. Sometimes it is convenient to use the *specific volume* $v = 1/\rho$ instead of the mass density. We will make the reader aware of such situations. The physical quantities depend on time $t \in \mathbb{R}_{\geq 0}$ and space $x \in \mathbb{R}$. In regular points of the bulk phases the fluid is described using the (one dimensional) isothermal Euler equations (3.1) and (3.2) introduced in 2.4.2, i.e.

$$\begin{aligned} \partial_t \rho + \partial_x(\rho u) &= 0, \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) &= 0. \end{aligned}$$

The Riemann initial data is given by (3.55)

$$\rho(x,0) = \begin{cases} \rho_V, \ x < 0 \\ \rho_L, \ x > 0 \end{cases} \quad \text{and} \quad u(x,0) = \begin{cases} u_V, \ x < 0 \\ u_L, \ x > 0 \end{cases}.$$

We have the jump conditions (3.3) and (3.4) across discontinuities

$$\begin{aligned} [\![\rho(u-W)]\!] &= 0, \\ \rho(u-W)\,[\![u]\!] + [\![p]\!] &= 0. \end{aligned}$$

Furthermore every discontinuity satisfies the entropy inequality (3.5)

$$\rho(u-W)\left[\!\left[g + e^{kin}\right]\!\right] \leq 0.$$

The quantity W is the speed of the discontinuity and $Z = -\rho(u-W)$ the mass flux where we will distinguish between a classical shock wave and the phase boundary (non-classical shock)

$$Z = \begin{cases} Q, & \text{shock wave} \\ z, & \text{phase boundary} \end{cases} \quad \text{and} \quad W = \begin{cases} S, & \text{shock wave} \\ w, & \text{phase boundary} \end{cases}.$$

The pressure p is linked to the mass density ρ via the EOS. We have for the mass density $\rho \in \Omega_\rho \subseteq (0,\infty)$. This domain can be split into the liquid, spinodal and vapor region, i.e. $\Omega_\rho = \Omega_{liq} \cup \Omega_{spin} \cup \Omega_{vap}$. Accordingly the EOS consists of three corresponding parts, i.e. an EOS for the vapor phase, the liquid phase and an intermediate part, see also Section 1.4. In the regular phases the EOS has the properties discussed in Section 1.3 or Section 3.1. As noted in Section 1.4 the (unphysical) intermediate part is characterized by the relation

$$\left(\frac{\partial p}{\partial v}\right)_T > 0.$$

and thus the considered Euler system becomes elliptic inside this region. We consider Riemann initial data which may be given as in (3.55), (3.59) or (3.60). Beside the well known numerical problems of hyperbolic equations (e.g. [56, 78]), we encounter further difficulties at a phase boundary. To solve a PDE numerically one usually uses a discretisation of the domain called mesh or grid. Then one may apply a *finite difference* approach and use the point values at the grid points to approximate the solution. Alternatively one may also use a *finite volume* approach where cell averages are used instead of point values. We will use methods based on the latter one. The averaging inside a cell causes the first problem, see Figure 4.1. Assume that at some time t the position of the phase boundary coincides with a cell boundary. In the (most likely) case that the phase boundary moves with the velocity $w \neq 0$ the phase boundary will have traveled the distance $w\Delta t$

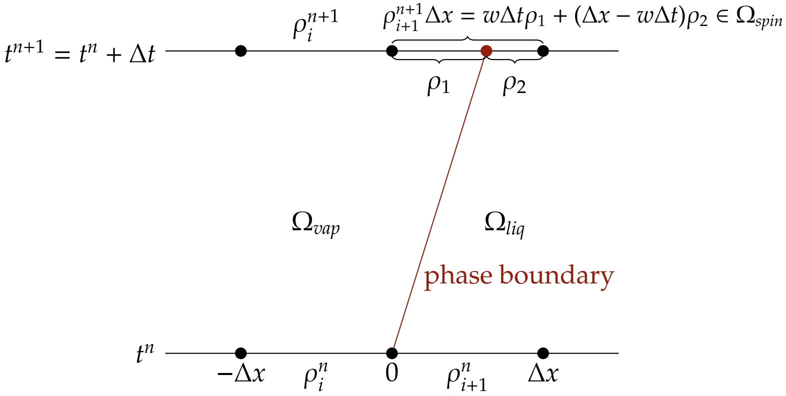

Figure 4.1: Sketch of the situation leading a wrong average. At t^n the densities are inside the pure phases. At t^{n+1} the phase boundary has moved by $w\Delta t$ and the averaged density ρ_{i+1}^{n+1} is now inside the spinodal region Ω_{spin}.

after the time step Δt. Thus the phase boundary will lie inside a cell. Now averaging can lead to unphysical states in Ω_{spin} and hence this will result in a wrong solution.
The second crucial point is the calculation of the quantities inside the star region. The quantities we want to determine are the values of the vapor phase ρ_V^*, v_V^*, p_V^*, the values of the liquid phase ρ_L^*, v_L^*, p_L^* and the speed of the phase boundary w. We would like to do this with sufficient accuracy, yet minimizing the computational costs. Finally we need to determine the correct flux (since we have two different phases) using the solution of the Riemann problem.

4.2 Numerical Method

In this section we want to present the numerical method we use to solve the stated problem in one space dimension. For compressible two phase flows with a sharp interface and a pressure jump at the interface there is not much literature available. A promising finite volume method for two dimensions was recently presented in the work by Chalons et al. [14]. The authors develop a conservative method which exactly resolves planar phase boundaries. A feature that yet is missing is the ability to treat nucleation and cavitation. Our method uses similar ideas in one space dimension and is able to treat nucleation and cavitation. Further results may be found in the works by Schleper [74] and Fechter et al. [31, 32]. For further literature we refer to the references therein.

The key idea of our approach is to use *Godunov's method* where the fluxes at cell interfaces between cells with equal phase may be calculated with any Riemann solver, see [78]. The flux at the phase boundary will be discussed later on. Concerning the discretization we for now follow the presentation and the notation given in [78]. The spatial domain $[a, b]$ is discretized in N cells $I_i, i = 1, \ldots, N$ of uniform size Δx with the cell boundaries $x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}$ and the cell center x_i, i.e.

$$\begin{cases} I_i &= [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}], \\ \Delta x &= |I_i| = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}} = \dfrac{b-a}{N}, \qquad i = 1, \ldots, N. \\ x_{i-\frac{1}{2}} &= (i-1)\Delta x,\ x_i = \left(i - \frac{1}{2}\right)\Delta x \end{cases} \tag{4.1}$$

The assumption of an uniform grid is just made for the sake of simplicity in the introduction and is basically not needed. We discretize the time interval $[0,T]$ using variable time steps Δt. The time step is restricted using the *CFL-condition*

$$\Delta t \leq C_{CFL} \frac{\Delta x}{S^n_{max}}. \tag{4.2}$$

The constant C_{CFL} is the *CFL-number* which is usually chosen in $(0,1]$. With S^n_{max} we denote the maximum absolute wave speed obtained in every time step during the numerical simulation. Given a function $\mathbf{U}(t,x)$ we calculate the cell average inside the computational cell I_i at time t^n as follows

$$\mathbf{U}^n_i = \frac{1}{|I_i|} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \mathbf{U}(t^n,x)\,\mathrm{d}x. \tag{4.3}$$

Once all the cell averages are calculated the key idea of Godunov was to solve the PDE by solving the Riemann problems at each cell boundary and use the obtained solution to advance in time. This highlights the importance of Riemann problems, since they are crucial building blocks in numerical methods for hyperbolic problems. The self-similar solution of the Riemann problem between the cells I_{i-1} and I_i at $x_{i-1/2}$ is given by $\mathbf{U}_{i-1/2}(t,x) = \mathbf{U}_{i-1/2}(x/t)$. Analogously we denote the solution at the right cell interface $x_{i+1/2}$ between the cells I_i and I_{i+1} by $\mathbf{U}_{i+1/2}(x/t)$. The flux at $x_{i-1/2}$ between the cells I_{i-1} and I_i is denoted by $\mathbf{F}_{i-1/2}$. Accordingly the flux at $x_{i+1/2}$ between the cells I_i and I_{i+1} is denoted by $\mathbf{F}_{i+1/2}$. Written in *conservative form* Godunov's method then reads

$$\mathbf{U}^{n+1}_i = \mathbf{U}^n_i - \frac{\Delta t}{\Delta x}\left[\mathbf{F}_{i+\frac{1}{2}} - \mathbf{F}_{i-\frac{1}{2}}\right], \tag{4.4}$$

$$\mathbf{F}_{i+\frac{1}{2}} = \mathbf{F}\Big(\mathbf{U}_{i+\frac{1}{2}}(0)\Big). \tag{4.5}$$

An important progress in the development of numerical methods was made by the observation, that one does not have to solve the Riemann problem exactly to obtain a numerical solution of the PDE. This led to a variety of Riemann solvers which all try to retain as much structure as possible of the exact solution. One common approach is to approximate the solution $\mathbf{U}_{i+1/2}(0)$. Other methods directly compute an approximation of the flux between the cells. However, both use (4.4) to obtain the solution in the next time step. An overview can be found in the given literature and the references therein. In the case of a single phase Riemann problem we will mainly use the *HLL* solver in this work, see [42, 78]. However, one may use any standard Riemann solver away from the phase boundary[1].

4.2.1 Grid Alignment and Adaption

We now want to comment on the first stated difficulty that we pointed out in the context of two phase flows with a sharp interface. For this reason we assume that we have constant cell values $\mathbf{U}_i^n$ belonging to two different phases and that the phase boundaries are aligned with the cell boundaries. Let us focus on a single phase boundary moving at the velocity $w \neq 0$ located at a certain $x_{i_0+1/2}$. As explained in Section 4.1 the phase boundary will lie inside a cell at $t^{n+1} = t^n + \Delta t$ and hence averaging will lead to unphysical phase states. In order to avoid this situation we always align our grid to the phase boundary. This changes the size of the cells and thus we have to deal with different cell sizes. This is done in the following way. We move the cell boundary according to the phase boundary, i.e. $x_{i_0+1/2} = x_{i_0+1/2} + w\Delta t$, see Figure 4.2. Next we compare every cell to certain thresholds given by the average cell size $\Delta x_{av} := (b-a)/N$ and the two parameters ϵ_1 and ϵ_2. Now we adjust the grid according to the following rules. If a cell fulfills $\Delta x_i > \epsilon_1 \Delta x_{av}$ the cell is too large and we split it into two. If a cell fulfills $\Delta x_i < \epsilon_2 \Delta x_{av}$ the cell is to small and we merge it with a neighbouring cell, if both belong to the same phase. The cell values have to be updated accordingly. In the case of nucleation and cavitation we may encounter small cells that *must not* be

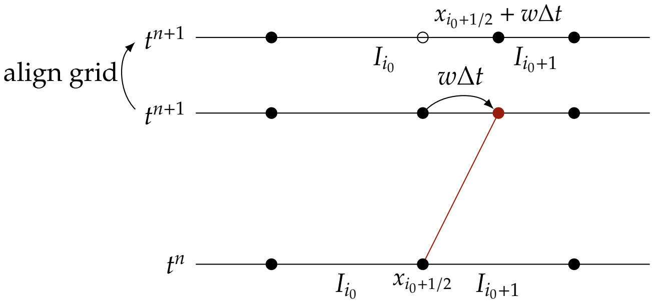

Figure 4.2: Align grid to the new position of the phase boundary.

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[1] We also tested the *exact Riemann solver* and the *Weighted Average Flux*, see [78]

merged with the neighbouring cells. How we deal with this situation will be explained later on.

Since cell sizes may change in every time step, we need to adjust equation (4.4) so that it is still in conservative form. The result reads

$$\mathbf{U}_i^{n+1} = \frac{\Delta x_i^n}{\Delta x_i^{n+1}} \mathbf{U}_i^n - \frac{\Delta t}{\Delta x_i^{n+1}} \left[\mathbf{F}_{i+\frac{1}{2}} - \mathbf{F}_{i-\frac{1}{2}} \right]. \tag{4.6}$$

with Δx_i^n and Δx_i^{n+1} being the cell sizes at the times t^n and t^{n+1}. One immediately verifies that (4.6) reduces to (4.4) for constant cell sizes. Further we calculate and update the time step as follows. The initial time step is obtained by using

$$S_{max}^0 = \max\{|u-a|, |u+a|\} \quad \text{and} \quad \Delta t = C_{CFL} \frac{\Delta x_0}{S_{max}^0}. \tag{4.7}$$

Where the maximum is computed considering all cell values. As the computation evolves we recalculate the time step as

$$\begin{aligned} \Delta x_{min} &= \min_{i=1,\dots,N} \{\Delta x_i \,|\, \Delta x_i \geq \epsilon_2 \Delta x_{av}\}, \\ S_{max}^n &= \max_S |S|, \\ \Delta t &= C_{CFL} \frac{\Delta x_{min}}{S_{max}^n}. \end{aligned} \tag{4.8}$$

It remains to discuss the case if a small cell of one phase is surrounded by cells of the other phase and thus must not be merged with its neighbours. This is the case when phase creation occurs [2]. In this case we proceed as follows. For cells with size $\Delta x_i < \epsilon_2 \Delta x_{av}$ we apply a *local time stepping method* as properly discussed by Müller and Stiriba [66]. We only need a simple reduced version of the method presented in [66] and will briefly present the used method in the following, see also Figure 4.3.
Let i_0 be the index of the small cell. We then consider the triplet $\{U_{i_0-1}, U_{i_0}, U_{i_0+1}\}$ and the corresponding quantities. Now we perform a time evolution starting at t^n with the small time steps $\Delta\tau$ until the final time $t^{n+1} = t^n + \Delta t$. The

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[2] It is further possible that this happens when two phase boundaries move towards each other and the enclosed phase might vanish. This situation is not considered here and will be discussed in the future.

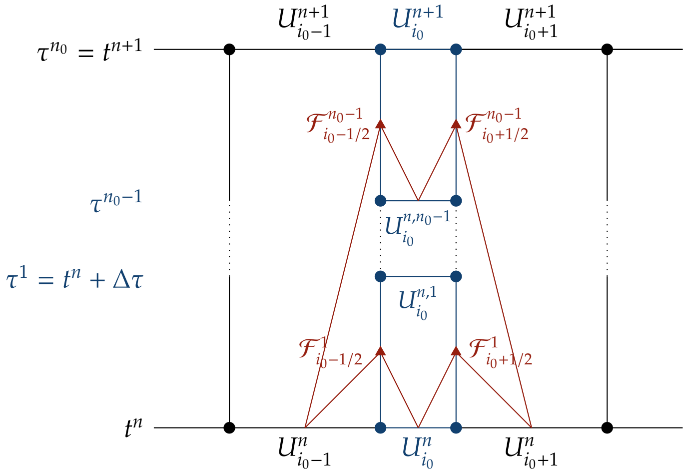


Figure 4.3: Simplified local time stepping for isolated small cells according to [66]

small cell is updated according to formula (4.6) with the time step $\Delta\tau$ and the fluxes $\mathcal{F}_{i_0\pm1/2}^{\nu}$ at the current time level $\tau^\nu = t^n + \nu\Delta\tau$ with $\nu = 0, \ldots, n_0$ and $\tau^{n_0} = t^{n+1}$ [3]. We have

$$\mathbf{U}_{i_0}^{n,\nu+1} = \frac{\Delta x_{i_0}^{\nu}}{\Delta x_{i_0}^{\nu+1}} \mathbf{U}_{i_0}^{n,\nu} - \frac{\Delta\tau}{\Delta x_{i_0}^{\nu+1}} \left[\mathcal{F}_{i_0+\frac{1}{2}}^{\nu} - \mathcal{F}_{i_0-\frac{1}{2}}^{\nu} \right]. \tag{4.9}$$

The values of the neighbouring cells remain unchanged throughout the time evolution. For the update of these (large) neighbouring cells we have to take care of the fluxes at $x_{i_0-1/2}$ and $x_{i_0+1/2}$. According to [66] this is done in the following way. At t^n we calculate the fluxes $\mathbf{F}_{i_0\pm1/2}$ as usual. At every further time level we update these fluxes as follows

$$\mathbf{F}_{i_0\pm1/2}^{\nu} = \mathbf{F}_{i_0\pm1/2}^{\nu-1} + \frac{\Delta\tau}{\Delta t} \mathcal{F}_{i_0\pm1/2}^{\nu}, \; \nu = 1, \ldots, n_0.$$

The fluxes obtained at the end of the evolution of the small cell may then be used in (4.6) to advance the neighbouring cells from t^n to t^{n+1}.

---

[3] A common choice is to choose $\Delta\tau = 2^{-n_0}\Delta t$ such that the *CFL-condition* on the fine level is satisfied, see [66].

4.2.2 Solution at the Interface

In the following we want to discuss the solution at the phase boundary. Therefore we rely on the results presented in the previous Chapter 3. The solution of the two phase Riemann problem consists of three waves, separating four constant states. In particular we are searching the values in the star region, i.e. ρ_V^*, p_V^*, u_V^* in the vapor phase, ρ_L^*, p_L^*, u_L^* in the liquid phase and the velocity w of the phase boundary or the mass flux z. The pressure and the density inside each phase are not independent from each other due to the EOS given for the particular phase. Further we know that the pressures at the interface are uniquely linked using equation (3.38), see Theorem 3.2.2. The mass flux is given by the kinetic relation (3.34)

$$z = \tau p_V \left[\!\left[g + e^{kin} \right]\!\right] = \tau p_V \left[g_L - g_V + e_L^{kin} - e_V^{kin} \right].$$

Thus according to Theorem 3.3.8 we have to solve the following system for (p_V^*, p_L^*) to obtain the complete solution

$$\mathbf{0} = \mathbf{G}(p_V^*, p_L^*) = \begin{pmatrix} [\![p]\!] + z^2 [\![v]\!] \\ f_V(p_V^*, \mathbf{W}_V) + f_L(p_L^*, \mathbf{W}_L) + z\,[\![v]\!] + \Delta u \end{pmatrix}. \tag{4.10}$$

The quantities in the second component are given as in Theorem 3.3.8, with the slight difference that we now explicitly use the liquid pressure. For the sake of completeness the Jacobian reads

$$\mathbf{DG}(p_V^*, p_L^*) = \dots$$
$$\begin{pmatrix} -1 + 2z\dfrac{\partial z}{\partial p_V^*}[\![v]\!] + z^2\left(\dfrac{v_V^*}{a_V^*}\right)^2 & 1 + 2z\dfrac{\partial z}{\partial p_L^*}[\![v]\!] - z^2\left(\dfrac{v_L^*}{a_L^*}\right)^2 \\ \dfrac{\mathrm{d}}{\mathrm{d}p_V^*} f_V(p_V^*, \mathbf{W}_V) + \dfrac{\partial z}{\partial p_V^*}[\![v]\!] + z\left(\dfrac{v_V^*}{a_V^*}\right)^2 & \dfrac{\mathrm{d}}{\mathrm{d}p_L^*} f_L(p_L^*, \mathbf{W}_L) + \dfrac{\partial z}{\partial p_L^*}[\![v]\!] - z\left(\dfrac{v_L^*}{a_L^*}\right)^2 \end{pmatrix}. \tag{4.11}$$

The derivatives of the classical wave functions are given as in Subsection 3.1.2 and the derivatives of the kinetic relation are as in Section 3.2.

Once we have determined the pressures we can calculate the densities via the corresponding EOS, the mass flux z via the kinetic relation, the velocities via the wave relations for the classical waves and the velocity of the phase boundary using the definition of the mass flux $z = -\rho(u - w)$. Since we always align the computational grid with the phase boundary we have to use the corresponding flux when we apply (4.6). The flux at the phase boundary is determined using the jump conditions (3.3) and (3.4). These may be rewritten as

$$\begin{aligned}\rho_V^*(u_V^* - w) &= \rho_L^*(u_L^* - w) = -z,\\ -zu_V^* + p_V^* &= -zu_L^* + p_L^*.\end{aligned}$$

Thus we directly see the flux across the phase boundary, i.e.

$$\mathbf{F}_{PB} = \begin{bmatrix} -z \\ -zu^* + p^* \end{bmatrix}. \tag{4.12}$$

Here one has the freedom to choose either the vapor or the liquid star state values.

So far we have discussed the case *with* phase transition. The case *without* phase transition is obtained using $z = 0$, which then implies $[\![p]\!] = 0$ and $[\![u]\!] = 0$. Thus we have to solve the single nonlinear equation given in Theorem 3.3.5. The flux is given by

$$\mathbf{F}_{PB} = \begin{bmatrix} 0 \\ p^* \end{bmatrix}. \tag{4.13}$$

Further one immediately verifies that in this case the phase boundary is quite analogue to a contact discontinuity. Therefore we use in our numerical simulations, for the case without phase transition, the wave speed estimates for the *HLLC* solver as given in [6, 78]. Given the (left) vapor state and the (right) liquid state we proceed as follows

$$\begin{aligned} S_L &= u_L + a_L,\\ S_V &= u_V - a_V,\\ w &= \frac{p_L - p_V + \rho_V u_V(S_V - u_V) - \rho_L u_L(S_L - u_L)}{\rho_V(S_V - u_V) - \rho_L(S_L - u_L)},\\ \rho_L^* &= \rho_L \frac{S_L - u_L}{S_L - w}. \end{aligned} \tag{4.14}$$

Here S_V and S_L denote the velocities of the classical waves. The density is calculated according to the HLLC solver as presented in [77, 78]. The pressure p^* may then be calculated using the liquid EOS. This procedure gives satisfactory results.

Due to the results in the previous chapter, especially Corollary 3.3.11, we use this simple calculation to choose proper initial pressure values for the Newton iteration in the case with phase transition.

4.3 Approximate Calculation of the Liquid Pressure

When we need to solve the Riemann problem at the phase boundary, we have to calculate the pressures in the star region by solving the nonlinear system (4.10). In numerical simulations this has to be done in every time step for possibly multiple phase boundaries. In the case without phase transition we remarked that it is possible to adapt the HLLC solver. This is a non-iterative Riemann solver which calculates the flux directly without any iteration. For one phase problems non-iterative Riemann solvers are widely used and very advanced, see [78]. The ultimate goal would be to give a reliable (and fast) non-iterative Riemann solver for the two phase Riemann problem. However, due to the presence of the phase boundary the situation is more complicated. Just to give an example, it is possible that the solution structure for one set of initial data may differ between the cases with and without phase transition. Thus it is not possible to easily predict the solution in the case with phase transition from the knowledge of the solution for the case without phase transition.

Nevertheless, we want to show that it is possible to reduce the system (4.10) to a single nonlinear equation by using a suited approximation of equation (3.38)

$$[\![p]\!] + z^2\,[\![v]\!] = 0.$$

However, we demand that the approximated liquid pressure also satisfies the properties given in Theorem 3.2.2, i.e.

(i) $p_L = p_V \quad \Leftrightarrow \quad p_L = p_V = p_0$,

(ii) $p_V < p_L$ for $p_V \neq p_0$,

(iii) p_L is a strictly monotone increasing function of p_V.

The key idea is to approximate (3.40) using a polynomial of second order at $p_L = p_0$, i.e.

$$\begin{aligned} h(p_V, p_L) &:= \tau \left[\!\!\left[g - \frac{1}{2} p (v_L + v_V) \right]\!\!\right] \\ &= \tau \left[g_L(p_L) - g_V(p_V) - \frac{1}{2}(p_L - p_V)(v_L(p_L) + v_V(p_V)) \right], \\ f(p_V, p_L) &:= [\![p]\!] + (p_V h(p_V, p_L))^2 [\![v]\!], \\ \tilde{f}(p_V, p_L) &:= f(p_V, p_0) + \partial_{p_L} f(p_V, p_0)(p_L - p_0) + \frac{1}{2}\partial^2_{p_L} f(p_V, p_0)(p_L - p_0)^2. \end{aligned} \tag{4.15}$$

For a suited p between p_L and p_0 we have

$$f(p_V, p_L) = \tilde{f}(p_V, p_L) + \frac{1}{6}\partial^3_{p_L} f(p_V, p)(p_L - p_0)^3.$$

Since (4.15) describes a quadratic polynomial in p_L we can directly calculate the two possible solutions of $0 = \tilde{f}(p_V, p_L)$

$$\tilde{\varphi}_\pm(p_V) = p_0 - \frac{\partial_{p_L} f(p_V, p_0)}{\partial^2_{p_L} f(p_V, p_0)} \pm \sqrt{\frac{\left(\partial_{p_L} f(p_V, p_0)\right)^2 - 2 f(p_V, p_0)\partial^2_{p_L} f(p_V, p_0)}{\left(\partial^2_{p_L} f(p_V, p_0)\right)^2}}. \tag{4.16}$$

Now there are three main tasks we have to deal with

(i) verify the correct root,

(ii) show that this root is well defined for all allowed temperatures and vapor pressures and

(iii) prove that the solution has the demanded properties.

The calculations for these questions are very technical and they quickly get out of hands. Therefore all the detailed calculations and derivatives which are needed here are given in the Appendix 9.2.

We start with the first question and determine the correct solution. This will be done by verifying the condition $p_0 = \tilde{\varphi}_\pm(p_0)$. We obtain the following

$$f(p_0, p_0) = 0, \quad \partial_{p_L} f(p_0, p_0) = 1 \quad \text{and} \quad \partial^2_{p_L} f(p_0, p_0) = 2\left(p_0 \partial_{p_L} h(p_0, p_0)\right)^2 [\![v]\!] < 0.$$

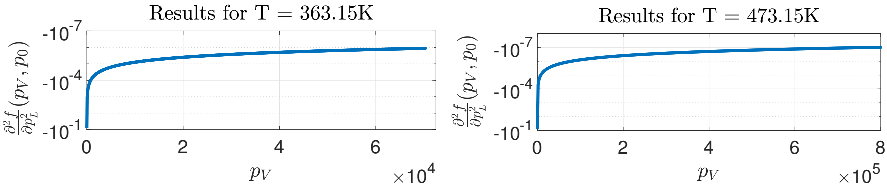
Inserting this into (4.16) gives

$$\tilde{\varphi}_{\pm}(p_0) = p_0 - \frac{1}{\partial^2_{p_L} f(p_V, p_0)} \pm \sqrt{\frac{1}{\left(\partial^2_{p_L} f(p_V, p_0)\right)^2}}.$$

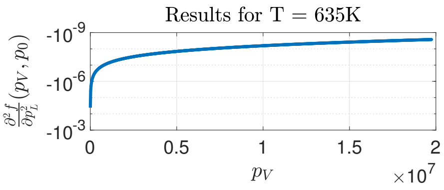
Since $\partial^2_{p_L} f(p_0, p_0)$ is negative the correct solution is given by $\tilde{\varphi}_{-}(p_0) = p_0$. Thus we write from now on

$$\tilde{\varphi}(p_V) := p_0 - \frac{\partial_{p_L} f(p_V, p_0)}{\partial^2_{p_L} f(p_V, p_0)} - \sqrt{\frac{\left(\partial_{p_L} f(p_V, p_0)\right)^2 - 2 f(p_V, p_0) \partial^2_{p_L} f(p_V, p_0)}{\left(\partial^2_{p_L} f(p_V, p_0)\right)^2}}. \tag{4.17}$$

Since the proof of the next two questions remains open, we briefly want to summarize the arguments that strongly suggest that these questions may be answered positively.
To show that the function (4.17) is well defined, we basically have to show that the appearing quotients depending on p_V are well defined. Numerical results *strongly* suggest that $\partial^2_{p_L} f(p_V, p_0) < 0$, see Figure 4.4.



(a) stiffened gas EOS, $T_0 = 363.15\,\mathrm{K}$ (b) linear Tait EOS, $T_0 = 473.15\,\mathrm{K}$



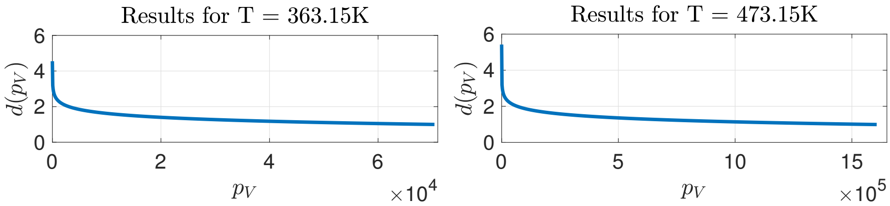
(c) non-linear Tait EOS, $T_0 = 635\,\mathrm{K}$

Figure 4.4: $\partial^2_{p_L} f(p_V, p_0)$ for different temperatures and EOS for the liquid phase.

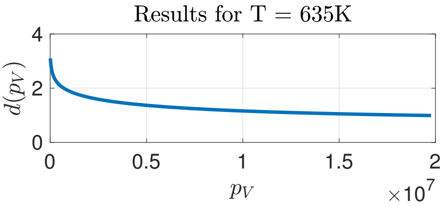
Thus it remains to show that

$$d(p_V) := \left(\partial_{p_L} f(p_V, p_0)\right)^2 - 2f(p_V, p_0)\partial^2_{p_L} f(p_V, p_0) > 0. \tag{4.18}$$

Again, numerical tests indicate that $d(p_V) > C > 0$, see Figure 4.5. Finally



(a) stiffened gas EOS, $T_0 = 363.15\,\mathrm{K}$ (b) linear Tait EOS, $T_0 = 473.15\,\mathrm{K}$



(c) non-linear Tait EOS, $T_0 = 635\,\mathrm{K}$

Figure 4.5: $d(p_V)$ for different temperatures and EOS for the liquid phase.

we have to verify that the properties of $\varphi(p_V)$ given in Theorem 3.2.2 also hold for the approximation (4.17). This has to be done for all allowed temperatures and the corresponding vapor pressure $p_V \in (0, \tilde{p}]$. Here $\tilde{p}$ is again the maximum vapor pressure at T_0 as defined in Chapter 3. The condition $p_0 = \tilde{\varphi}(p_0)$ is met as shown above. Further it is possible to prove that

$$\lim_{p_V \to 0} \tilde{\varphi}(p_V) = 0 \tag{4.19}$$

given that the EOS for the vapor phase is the ideal gas EOS[4]. The details are given in the Appendix 9.2. Further we have to show that $p_L = \tilde{\varphi}(p_V) > p_V$

---

[4] This is a purely mathematical consideration. Physically it needs to be discussed what really happens in the isothermal limit $p_V \to 0$.

for $p_V \neq p_0$. In view of the previous statements we suggest to investigate $\tilde{f}(p_V, p_V)$ and prove that it is negative for all $p_V \neq p_0$. Since (4.15) is (presumably) concave in p_L this would be sufficient. Finally we need to prove the monotonicity $\tilde{\varphi}'(p_V) > 0$. Due to the complexity, mostly caused by the high number of appearing terms, this is far from being solved. Nevertheless, numerical results again suggest that monotonicity holds. In Figures 4.6, 4.7 and 4.8 we present the function for the liquid pressure (4.17), the difference $p_L(p_V) - p_V$ and the relative error with respect to the solution obtained by solving (3.38) with a tolerance of $\varepsilon_{tol} = 10^{-9}$. From these results we see that the desired properties given in Theorem 3.2.2 hold. Let us finally remark that altogether it is more likely to prove these results if the ideal gas EOS is used for the vapor phase. In particular when it is used together with a linear EOS for the liquid phase. Many of the difficulties arise when p_V is close to zero. Therefore we also recommend to first try to prove the desired results for $p_V > \bar{p}$. A detailed choice has to be carefully discussed, but in our experience most problems already vanished for $\bar{p} = 1\,\text{Pa}$. For applications higher thresholds may also be possible, e.g. $\bar{p} = 100\,\text{Pa}$, which is approximately one sixth of the saturation pressure at 273.15 K.

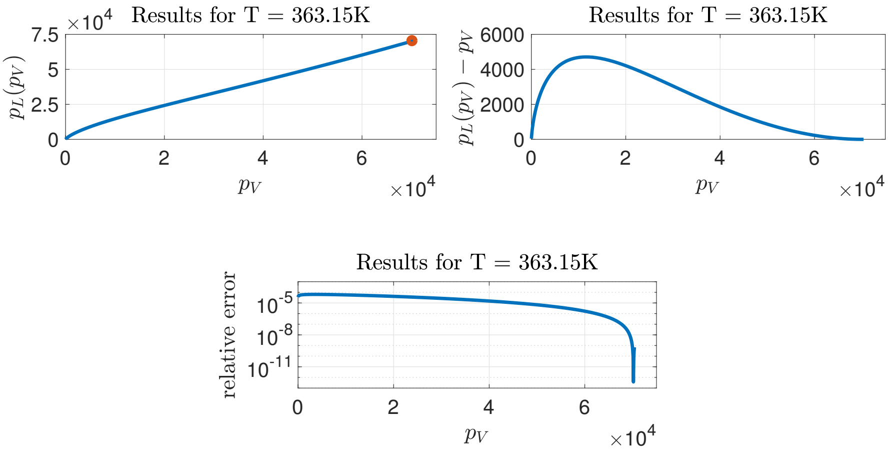


Figure 4.6: Results for the stiffened gas EOS at $T_0 = 363.15$ K.

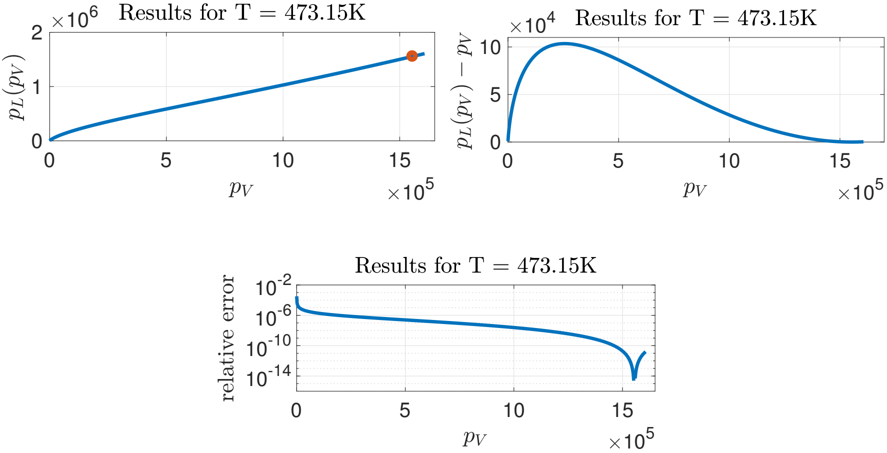


Figure 4.7: Results for the linear Tait EOS at $T_0 = 473.15$ K.

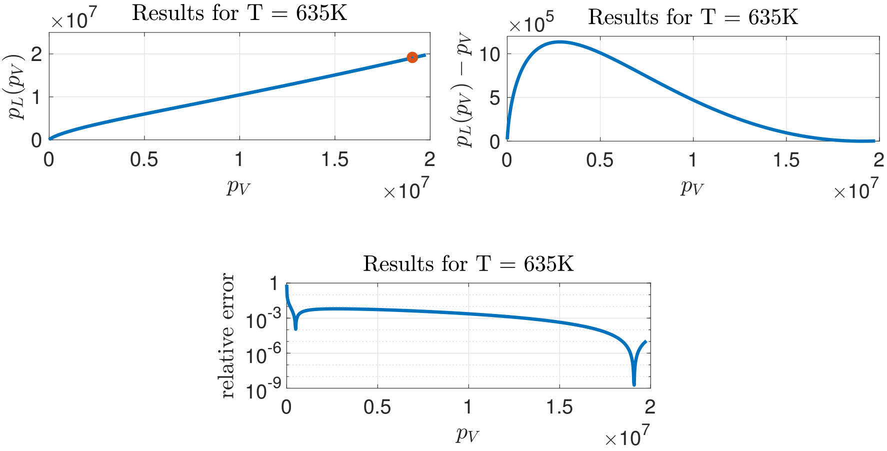


Figure 4.8: Results for the non-linear Tait EOS at $T_0 = 473.15$ K.

4.4 Phase Creation

The case of phase creation is a challenging issue since we not only have to detect when phase creation occurs. Further we also have to deal with technical problems like the creation of new cells which in most cases are very small and of course with multiple phase boundaries.

4.4.1 Cavitation

When we encounter a liquid/liquid Riemann Problem we may observe cavitation, i.e. the creation of vapor. The detailed analysis is presented in Subsection 3.4.2. In view of the results given there in Theorem 3.4.10, Definition 3.4.12 and Theorem 3.4.15 the main outline for the numerics is as follows. We solve the single phase Riemann Problem in the liquid phase. If there is no solution to this problem, in particular when the liquid pressure in the star region is smaller than the predefined minimum liquid pressure, $p^* < p_{min}$, we have cavitation. In this case we store the position of the involved cells and perform an extra calculation. Summarized the performed steps are as follows:

(i) Solve the single phase Riemann problem, if $p^* < p_{min}$ cavitation occurs.

(ii) Solve the single phase Riemann problem according to Theorem 3.4.15.[5]

(iii) From the solution we obtain p_V^*, z, w_{left} and w_{right}.

(iv) Create a vapor cell of size $(w_{right} - w_{left})\Delta t$ with the cell values ρ_V^*, p_V^* and u_V^*.

(v) The fluxes at the phase boundaries are given by

$$\mathbf{F}_{PB}^{(left)} = \begin{bmatrix} z \\ -zu_V^* + p_V^* \end{bmatrix} \quad \text{and} \quad \mathbf{F}_{PB}^{(right)} = \begin{bmatrix} -z \\ -zu_V^* + p_V^* \end{bmatrix}. \tag{4.20}$$

In the next time step we then have two phase boundaries which are treated as discussed in Section 4.2.

---

[5] For the solution one may also use the approximation presented in Section 4.3

4.4.2 Nucleation

The case of nucleation is treated analogous to the previous case of cavitation. When we encounter a vapor/vapor Riemann Problem we may observe nucleation, i.e. the creation of liquid. The detailed analysis is presented in Subsection 3.4.1. In view of the results given there in Theorem 3.4.1, Definition 3.4.2 and Theorem 3.4.6 the main outline for the numerics is as follows. We solve the single phase Riemann Problem in the vapor phase. If there is no solution to this problem, i.e. when the vapor pressure in the star region is greater than the predefined maximum vapor pressure, $p^* > \tilde{p}$, we have nucleation. In this case we store the position of the involved cells and perform an extra calculation. Summarized the performed steps are as follows:

(i) Solve the single phase Riemann problem, if $p^* > \tilde{p}$ nucleation occurs.

(ii) Solve the single phase Riemann problem according to Theorem 3.4.6

(iii) From the solution we obtain p^*_L, z, w_{left} and w_{right}.

(iv) Create a liquid cell of size $(w_{right} - w_{left})\Delta t$ with the cell values ρ^*_L, p^*_L and u^*_L.

(v) The fluxes at the phase boundaries are given by

$$\mathbf{F}^{(left)}_{PB} = \begin{bmatrix} -z \\ -zu^*_L + p^*_L \end{bmatrix} \quad \text{and} \quad \mathbf{F}^{(right)}_{PB} = \begin{bmatrix} z \\ -zu^*_L + p^*_L \end{bmatrix} \tag{4.21}$$

Again, in the next time step we then have two phase boundaries which are treated as discussed in Section 4.2. Especially in the case of nucleation it is important to not that the created cells are usually very small (e.g. seven orders of magnitude) compared to the other cells. Thus the local time stepping presented in Section 4.2 is very much needed to avoid too small time steps in the whole computational domain. We will again comment on this in the following Section 4.5

4.5 Numerical Examples

In this section we want to present and discuss examples of two phase flow problems as discussed in the previous Sections 4.2 and 4.4. As before we will first discuss cases with two phase initial data followed by examples exhibiting nucleation and cavitation. All the results of the numerical calculations are compared to the solution of the Riemann problem obtained with Newtons method using the tolerance $\varepsilon_{tol} = 10^{-9}$. More precisely, since in some cases the standard Newton method failed to converge, we used the *Newton-Armijo* method as presented in Kelley [49]. The saturation pressure is calculated using the steam tables [84]. In order to distinguish the phases we proceed according to the examples in Section 3.5, see equations (3.63) and (3.65). If not stated otherwise we used the exact solution of the Riemann problem at the phase boundary in our numerical calculations [6]. Using this approach we obtained satisfactory results.

4.5.1 Two Phase Initial Data

Here we present examples for initial two phase data. Therefore we use the data given in [37].

Example 1

The first example is given by the initial data as given in Table 4.1 and corresponds to *Example 1* in [37]. The following computation was performed

	p_V	u_V	p_L	u_L
Initial Data	2300 Pa	$-100\,\frac{\mathrm{m}}{\mathrm{s}}$	1000 Pa	$100\,\frac{\mathrm{m}}{\mathrm{s}}$

	T_0	p_0
Saturation Values	293.15 K	2339.215Pa

Table 4.1: Initial Data - Example 1

---

[6] There are mainly two reasons why we omit a presentation of numerical examples using the approximation for the liquid pressure (4.17). First there where only very small quantitative differences in the solution, compared to the case with the exact Riemann solution at the phase boundary, for the considered pressure and temperature ranges. This emphasizes the conjectured accuracy of the approximation as it also can be seen in the given figures. Further we obtained no significant speed up of our calculations. These reasons, together with the fact that we have no analytical proof for the correctness of the approximation, led to the decision to only present examples with the exact Riemann solution at the phase boundary. However, the interest in a reliable and fast non-iterative Riemann solver at the phase boundary remains and the approximation may be a first step in this direction.

with the linear Tait EOS and the parameters

$$\Delta t = 2.850985 \cdot 10^{-6}\,\mathrm{s},\ \Delta x_0 = 0.5 \cdot 10^{-2}\,\mathrm{m},\ C_{CFL} = 0.9,$$
$$t_{end} = 10^{-3}\,\mathrm{s} \text{ and } x \in [-2, 2]\,\mathrm{m}.$$

The size of the time step is calculated as given in (4.7), (4.8) and we calculated 497 time steps. The phases are distinguished using the values given in Table 4.2. In Figure 4.9 the numerical results for the case with phase transition are shown. For the numerical solution we used the HLL solver as in [78]. The values in the star region are given in Table 4.3.

$\tilde{p}$	$\tilde{\rho}$	p_{min}	ρ_{min}
2339.618586 Pa	0.017293 $\frac{\mathrm{kg}}{\mathrm{m}^3}$	0 Pa	998.176933 $\frac{\mathrm{kg}}{\mathrm{m}^3}$

Table 4.2: Maximum vapor pressure and corresponding quantities for the linear Tait EOS together with the ideal gas EOS at $T_0 = 293.15\,\mathrm{K}$

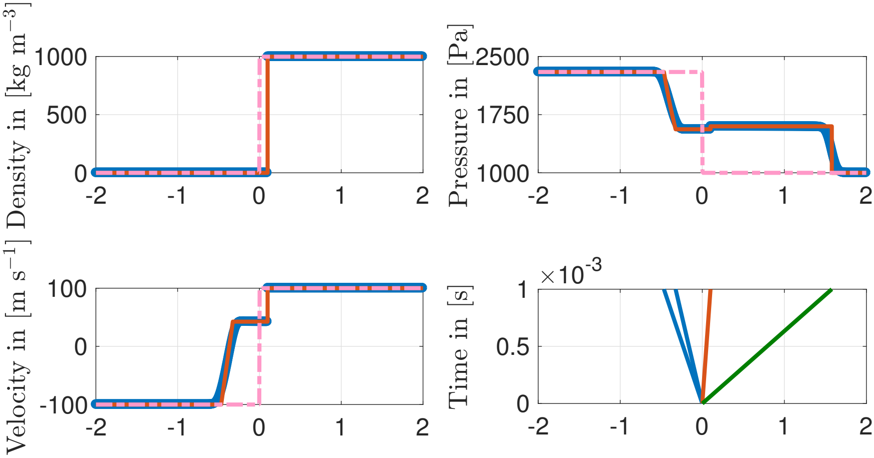


Figure 4.9: **Solution - Example 1:** magenta: initial data, red: exact solution, blue: numerical solution; wave structure: rarefaction wave (blue), phase boundary (red) and shock wave (green)

vapor	p_V^*	u_V*
exact	1561.366723 Pa	42.475926 $\frac{\mathrm{m}}{\mathrm{s}}$
numerical	1559.901001 Pa	42.347724 $\frac{\mathrm{m}}{\mathrm{s}}$
liquid	p_L^*	u_L^*
exact	1599.555352 Pa	100.000406 $\frac{\mathrm{m}}{\mathrm{s}}$
numerical	1598.226735 Pa	100.000405 $\frac{\mathrm{m}}{\mathrm{s}}$

Table 4.3: Solution Data - Example 1

Example 2

The initial data for the second example is given in Table 4.4 and corresponds to *Example 2* in [37]. The following computation was performed with the linear Tait EOS and the parameters

	p_V	u_V	p_L	u_L
Initial Data	60000 Pa	-200 $\frac{\mathrm{m}}{\mathrm{s}}$	100000 Pa	-50 $\frac{\mathrm{m}}{\mathrm{s}}$

	T_0	p_0
Saturation Values	473.15 K	1554671.86827Pa

Table 4.4: Initial Data - Example 2

$$\Delta t = 3.769159 \cdot 10^{-6}\,\mathrm{s},\ \Delta x_0 = 0.5 \cdot 10^{-2}\,\mathrm{m},\ C_{CFL} = 0.9,$$
$$t_{end} = 10^{-3}\,\mathrm{s} \text{ and } x \in [-2, 2]\,\mathrm{m}.$$

The time step is calculated as given in (4.7) and (4.8). We calculated 373 time steps. The phases are distinguished using the values given in Table 4.5. In Figure 4.10 the numerical results for the case with phase transition are shown. For the numerical solution we used the HLL solver as in [78].

$\tilde{p}$	$\tilde{\rho}$	p_{min}	ρ_{min}
1606360.89173 Pa	7.356189 $\frac{\mathrm{kg}}{\mathrm{m}^3}$	0 Pa	863.494296 $\frac{\mathrm{kg}}{\mathrm{m}^3}$

Table 4.5: Maximum vapor pressure and corresponding quantities for the linear Tait EOS together with the ideal gas EOS at $T_0 = 473.15\,\mathrm{K}$

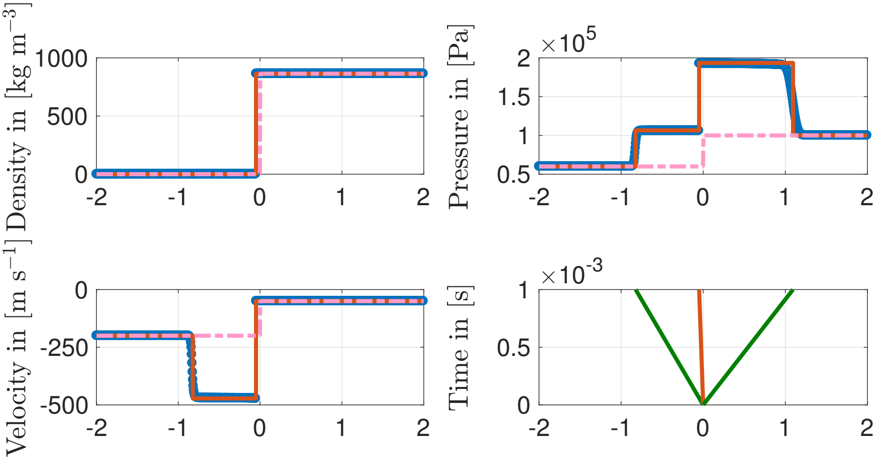


Figure 4.10: **Solution with Phase Transition - Example 2:** magenta: initial data, red: exact solution, blue: numerical solution; wave structure: two shock waves (green), phase boundary (red)

The values in the star region are given in Table 4.6. Note that for this

vapor	p_V^*	u_V*
exact	106525.049799 Pa	$-471.944614\ \frac{\mathrm{m}}{\mathrm{s}}$
numerical	106010.212128 Pa	$-472.609211\ \frac{\mathrm{m}}{\mathrm{s}}$
liquid	p_L^*	u_L^*
exact	193463.627097 Pa	$-49.905389\ \frac{\mathrm{m}}{\mathrm{s}}$
numerical	192800.859460 Pa	$-49.906060\ \frac{\mathrm{m}}{\mathrm{s}}$

Table 4.6: Solution Data - Example 2

example the wave structure changes between the cases with and without phase transition, see exemplary Figure 4.11.

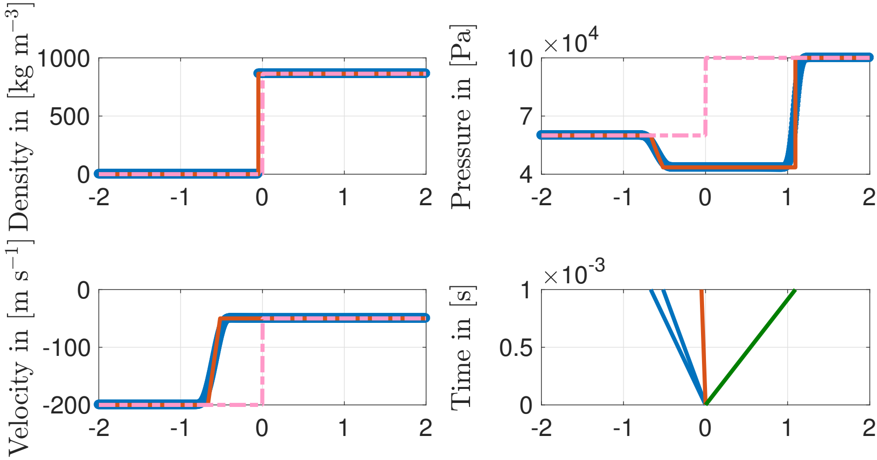


Figure 4.11: **Solution without Phase Transition - Example 2:** magenta: initial data, red: exact solution, blue: numerical solution; wave structure: rarefaction wave (blue), phase boundary (red), shock wave (green)

4.5.2 Phase Creation

Example 3

The third example is a nucleation test case with the initial data as given in Table 4.7 and it corresponds to *Example 3* in [37]. The following computation

	p_V^-	u_V^-	p_V^+	u_V^+
Initial Data	70000 Pa	$2.7\,\frac{\text{m}}{\text{s}}$	70000 Pa	$-2.7\,\frac{\text{m}}{\text{s}}$

	T_0	p_0
Saturation Values	363.15 K	70182.360745 Pa

Table 4.7: Initial Data - Example 3

was performed with the linear Tait EOS and the parameters

$$\Delta t = 1.091991 \cdot 10^{-5}\,\text{s},\ \Delta x_0 = 0.5 \cdot 10^{-2}\,\text{m},\ C_{CFL} = 0.9,$$
$$t_{end} = 10^{-3}\,\text{s and } x \in [-2, 2]\,\text{m}.$$

The time step is calculated as given in (4.7) and (4.8). The phases are distinguished using the values given in Table 4.8. It is important to note, that we connected the EOS linearly with respect to the density. If we instead connect the two EOS linearly with respect to the volume no nucleation would occur, due to a larger value of $\tilde{p}$, see Table 4.9. To calculate these quantities we use Definition 1.4.1 with $v_m = v_L(p_{min}) = 1/\rho_{min}$

$\tilde{p}$	$\tilde{\rho}$	p_{min}	ρ_{min}
70388.660656 Pa	0.419977 $\frac{\text{kg}}{\text{m}^3}$	0 Pa	965.289008 $\frac{\text{kg}}{\text{m}^3}$

Table 4.8: Maximum vapor pressure and corresponding quantities for the linear Tait EOS together with the ideal gas EOS at $T_0 = 363.15\,\text{K}$

$$\begin{aligned} 0 &= p_0\,(v_{0,V} - v_{0,L}) - \dots \\ &- \left(\int_{v_{0,L}}^{v_m} p_L(v)\,\mathrm{d}v + \frac{1}{2}\,(p_V(\tilde{v}) + p_{min})\,(\tilde{v} - v_m) + \int_{\tilde{v}}^{v_{0,V}} p_V(v)\,\mathrm{d}v\right). \end{aligned} \tag{4.22}$$

Once the EOS for the liquid and the vapor phase are specified, equation (4.22) can be solved for $\tilde{v}$. Figure 4.12 shows the numerical results for the case with phase transition. For the numerical solution we used the HLL solver as in [78]. Note for the wave structure, that the phase boundaries are so close that they cannot be distinguished in the given picture. The values are

$\tilde{p}$	$\tilde{\rho}$	p_{min}	ρ_{min}
115702.332624 Pa	0.690343 $\frac{\text{kg}}{\text{m}^3}$	0 Pa	965.289008 $\frac{\text{kg}}{\text{m}^3}$

Table 4.9: Alternative maximum vapor pressure and corresponding quantities for the linear Tait EOS together with the ideal gas EOS at $T_0 = 363.15\,\text{K}$

$$w_{\text{left/right}} = \pm 0.000203\,\frac{\text{m}}{\text{s}} \quad \text{and thus} \quad (w_{right} - w_{left}) \cdot t_{end} = 4.06 \cdot 10^{-7}\,\text{m}.$$

The values in the star region [7] for the pressure are given in Table 4.10. The

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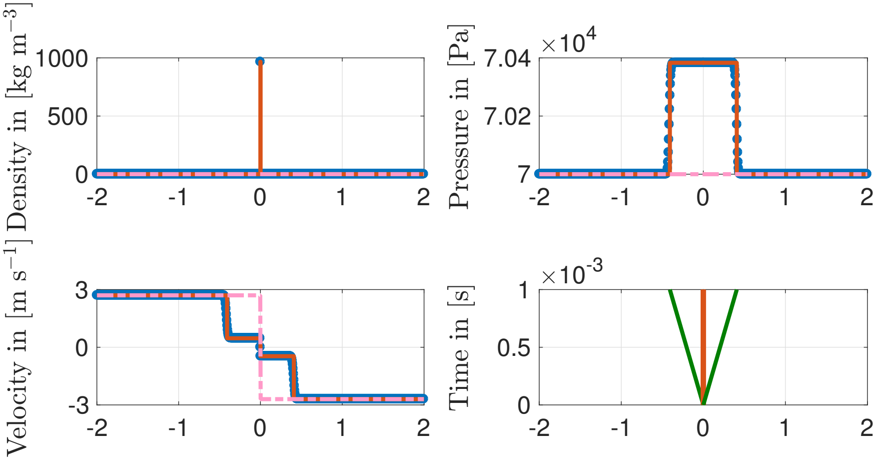
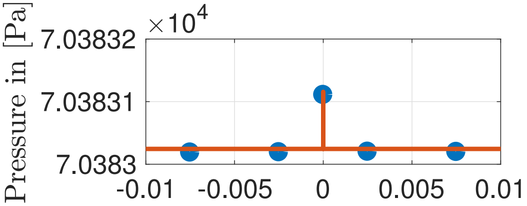
[7] Note that due to numerical errors there is a small difference of $\Delta p \approx 7.95 \cdot 10^{-4}$ Pa in the vapor pressures in the star region. This difference is negligible with respect to the magnitude of the present vapor pressure.



(a) magenta: initial data, red: exact solution, blue: numerical solution; wave structure: shock waves (green) and phase boundaries (red)



(b) Detailed zoom for the pressure; red: exact solution, blue: numerical solution

Figure 4.12: **Solution - Example 3**

	$p_V^{*,-}$	p_L^*	$p_V^{*,+}$
exact	70383.024449 Pa	70383.115685 Pa	70383.024449 Pa
numerical	70383.019144 Pa	70383.110613 Pa	70383.019939 Pa

Table 4.10: Solution Data (Pressure) - Example 3

values for the velocity in the star region[8] are given in Table 4.11. To treat

---

[8] As for the pressures we have a small difference of order 10^{-6} in the absolute values of the vapor velocities in the star region.

	$u_V^{*,-}$	u_L^*	$u_V^{*,+}$
exact	$0.466005\ \frac{\mathrm{m}}{\mathrm{s}}$	$0\ \frac{\mathrm{m}}{\mathrm{s}}$	$-0.466005\ \frac{\mathrm{m}}{\mathrm{s}}$
numerical	$0.465993\ \frac{\mathrm{m}}{\mathrm{s}}$	$-0.223424 \cdot 10^{-5}\ \frac{\mathrm{m}}{\mathrm{s}}$	$-0.465997\ \frac{\mathrm{m}}{\mathrm{s}}$

Table 4.11: Solution Data (Velocity) - Example 3

the nucleation case we apply the local time stepping as presented before in Section 4.2, see equation (4.9) and Figure 4.3. The cell size of the liquid phase after it is created is

$$\Delta x_L = 4.429422 \cdot 10^{-9}\,\mathrm{m}.$$

Together with a local CFL-number of $C_{CFL} = 0.5$ this leads to an initial local time step of the size $\Delta\tau = 5.4004 \cdot 10^{-12}\,\mathrm{s}$. Hence we have $\Delta\tau/\Delta t \approx 5 \cdot 10^{-7}$. For the first time step a total of 5093567 local time steps were performed [9].

Example 4

Next we present examples exhibiting cavitation. The initial data for example four is given in Table 4.12 and it corresponds to *Example 4* in [37]. The following computation was performed with the linear Tait EOS and the parameters

	p_L^-	u_L^-	p_L^+	u_L^+
Initial Data	60000 Pa	$-40\ \frac{\mathrm{m}}{\mathrm{s}}$	60000 Pa	$40\ \frac{\mathrm{m}}{\mathrm{s}}$

	T_0	p_0
Saturation Values	363.15 K	70182.360745 Pa

Table 4.12: Initial Data - Example 4

$$\Delta t = 2.961190 \cdot 10^{-6}\,\mathrm{s},\ \Delta x_0 = 0.5 \cdot 10^{-2}\,\mathrm{m},\ C_{CFL} = 0.9,$$
$$t_{end} = 10^{-3}\,\mathrm{s} \text{ and } x \in [-2, 2]\,\mathrm{m}.$$

---

[9] The calculation time of a simulation until $t_{end} = 10^{-3}\,\mathrm{s}$ is about 641514.65 s ≈ 7.5 d. For the simulation until $t_{end} = \Delta t \approx 2 \cdot 10^{-5}\,\mathrm{s}$ the calculation took 31828.89637 s ≈ 9 h. Both calculation times were obtained with *Matlab 2017a* running on a 64-Bit Linux OS with a *Intel® Xeon® CPU E5-2650 v4* with 2.20 GHz.

The time step is calculated as given in (4.7) and (4.8). The phases are distinguished using the values given in Table 4.8. The numerical results are presented in Figure 4.13 and we performed 476 time steps. For the numerical solution we used the HLL solver as in [78]. Note for the wave structure, that the head and tail speeds of the rarefaction waves are so close that they cannot be distinguished in the given picture. The values are

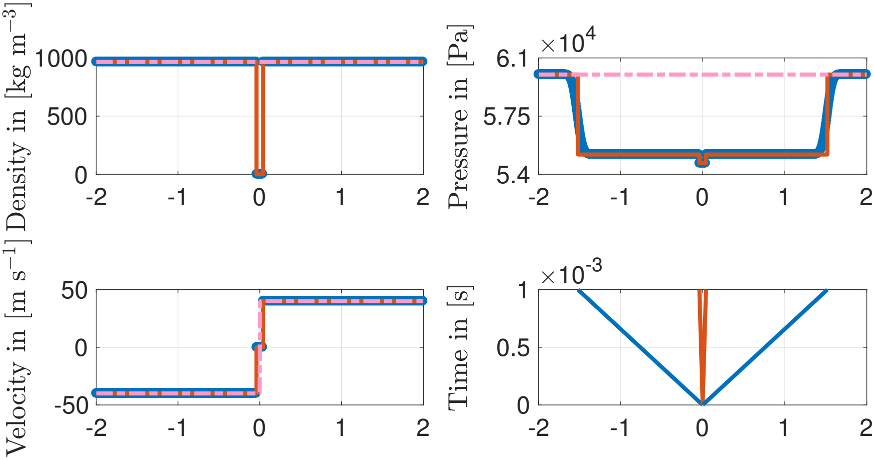


Figure 4.13: **Solution - Example 4:** magenta: initial data, red: exact solution, blue: numerical solution; wave structure: rarefaction waves (blue) and phase boundaries (red)

$$S^{\pm}_{head} = \pm 1519.659189\,\frac{\mathrm{m}}{\mathrm{s}},\; S^{\pm}_{tail} = \pm 1519.655820\,\frac{\mathrm{m}}{\mathrm{s}} \quad \text{and}$$

$$\left|S^{\pm}_{head} - S^{\pm}_{tail}\right| = 0.003369\,\frac{\mathrm{m}}{\mathrm{s}}.$$

The values in the star region [10] for the pressure are given in Table 4.13. The values for the velocity in the star region [11] are given in Table 4.14. To treat

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[10] Note that, as in the nucleation case, due to numerical errors there is a small difference in the liquid pressures in the star region. Thus there are also different values for the vapor pressure. In Table 4.13 we give the vapor pressure at the left phase boundary, the value at the right phase boundary is $p^*_V = 54666.652586$ Pa. Hence the difference is $\Delta p^*_V \approx 8.2 \cdot 10^{-5}$ Pa and thus it is negligible compared to the magnitude of the present pressure values.

[11] Similar to the pressure we have the following precise values for the left velocities $u^{*,-}_L = -39.9966314780956088\,\frac{\mathrm{m}}{\mathrm{s}}$ and $u^{*,-}_V = 0.1223002731 \cdot 10^{-5}\,\frac{\mathrm{m}}{\mathrm{s}}$. On the right side we have $u^{*,+}_L = 39.996631476453331\,\frac{\mathrm{m}}{\mathrm{s}}$ and $u^{*,+}_V = -0.229005314 \cdot 10^{-6}\,\frac{\mathrm{m}}{\mathrm{s}}$.

	$p_L^{*,-}$	p_V^*	$p_L^{*,+}$
exact	55188.614355 Pa	54666.652641 Pa	55188.614355 Pa
numerical	55188.613219 Pa	54666.652668 Pa	55188.612945 Pa

Table 4.13: Solution Data (Pressure) - Example 4

	$u_L^{*,-}$	u_V^*	$u_L^{*,+}$
exact	$-39.996631\,\frac{\mathrm{m}}{\mathrm{s}}$	$0\,\frac{\mathrm{m}}{\mathrm{s}}$	$39.996631\,\frac{\mathrm{m}}{\mathrm{s}}$
numerical	$-39.996631\,\frac{\mathrm{m}}{\mathrm{s}}$	$0.122300 \cdot 10^{-5}\,\frac{\mathrm{m}}{\mathrm{s}}$	$39.996631\,\frac{\mathrm{m}}{\mathrm{s}}$

Table 4.14: Solution Data (Velocity) - Example 4

the cavitation case we also used the local time stepping as presented before in Section 4.2, see equation (4.9) and Figure 4.3. However, compared to the nucleation case the cell size of the vapor phase after it is created is much larger, i.e.

$$\Delta x_V = 2.369553 \cdot 10^{-4}\,\mathrm{m}.$$

During the simulation the local time stepping was applied 11 times with a total of 97 small time steps.

Example 5

Corresponding to *Example 5* in [37] we present another example exhibiting cavitation. The initial data for example five is given in Table 4.15 The following computation was performed with the linear Tait EOS and the parameters

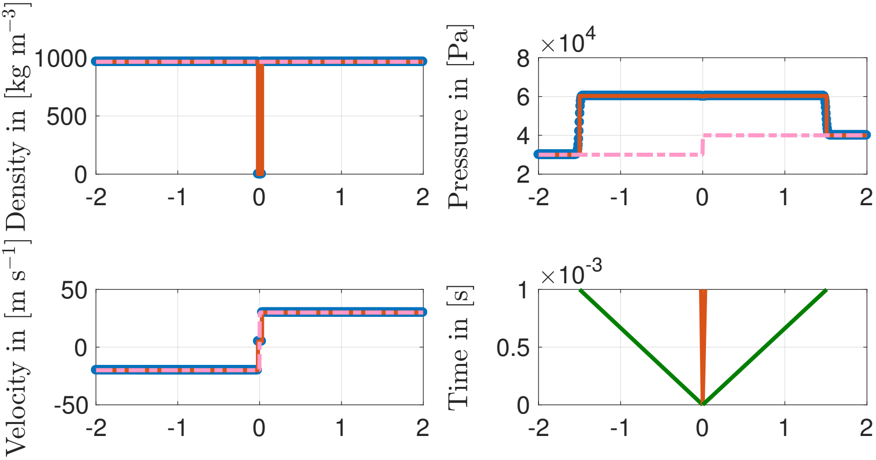
	p_L^-	u_L^-	p_L^+	u_L^+
Initial Data	30000 Pa	$-20\,\frac{\mathrm{m}}{\mathrm{s}}$	40000 Pa	$30\,\frac{\mathrm{m}}{\mathrm{s}}$

	T_0	p_0
Saturation Values	363.15 K	70182.360745 Pa

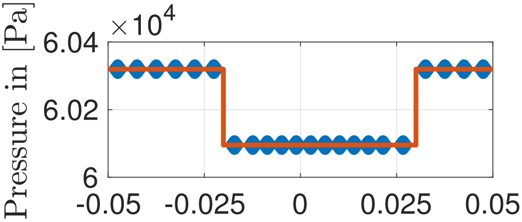
Table 4.15: Initial Data - Example 5

$$\Delta t = 2.980805 \cdot 10^{-6}\,\mathrm{s},\ \Delta x_0 = 0.5 \cdot 10^{-2}\,\mathrm{m},\ C_{CFL} = 0.9,$$
$$t_{end} = 10^{-3}\,\mathrm{s} \text{ and } x \in [-2, 2]\,\mathrm{m}.$$

The size of the time step is calculated as given in (4.7), (4.8) and we performed 492 time steps. Further the local time stepping was applied 19 times with a total of 180 small time steps. The phases are distinguished using the values given in Table 4.8. The numerical results are presented in Figure 4.14. Here we have exemplary used the *Weighted Average Flux* solver together with the *van Leer* limiter as in [78]. The values in the star region for the pressure are given in Table 4.16[12]. The values for the velocity in the star region are given



(a) magenta: initial data, red: exact solution, blue: numerical solution; wave structure: shock waves (green) and phase boundaries (red)



(b) Detailed zoom for the pressure; red: exact solution, blue: numerical solution

Figure 4.14: **Solution - Example 5**

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[12] As before there is a negligible difference in the numerical solution.

	$p_L^{*,-}$	p_V^*	$p_L^{*,+}$
exact	60319.800508 Pa	60095.298565 Pa	60319.800508 Pa
numerical	60319.798929 Pa	60095.298292 Pa	60319.799085 Pa

Table 4.16: Solution Data (Pressure) - Example 5

in Table 4.17.

	$u_L^{*,-}$	u_V^*	$u_L^{*,+}$
exact	$-20.021227\,\frac{\text{m}}{\text{s}}$	$4.996499\,\frac{\text{m}}{\text{s}}$	$30.014226\,\frac{\text{m}}{\text{s}}$
numerical	$-20.021227\,\frac{\text{m}}{\text{s}}$	$4.996599\,\frac{\text{m}}{\text{s}}$	$30.014226\,\frac{\text{m}}{\text{s}}$

Table 4.17: Solution Data (Velocity) - Example 5

Example 6

Example six is a modified version of example *RP-H5* given in [24]. The initial data is given in Table 4.18 The following computation was performed

	p_L^-	u_L^-	p_L^+	u_L^+
Initial Data	$2\cdot 10^6$ Pa	$-100\,\frac{\text{m}}{\text{s}}$	$2\cdot 10^6$ Pa	$100\,\frac{\text{m}}{\text{s}}$

	T_0	p_0
Saturation Values	437.310570 K	686358.293543 Pa

Table 4.18: Initial Data - Example 6

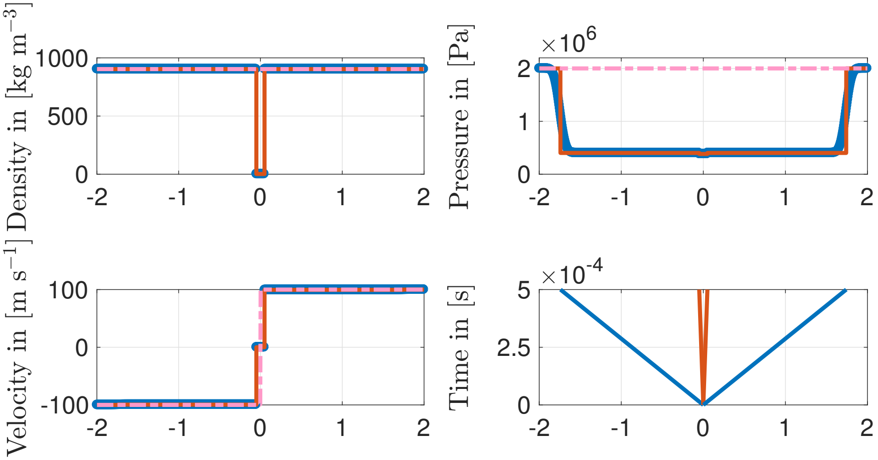
with the non-linear Tait EOS and the parameters

$$\Delta t = 1.291544\cdot 10^{-6}\,\text{s},\ \Delta x_0 = 0.5\cdot 10^{-2}\,\text{m},\ C_{CFL} = 0.9,$$
$$t_{end} = 5\cdot 10^{-4}\,\text{s and } x \in [-2,2]\,\text{m}.$$

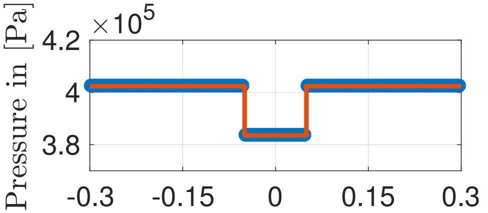
The time step is calculated as given in (4.7) and (4.8). The phases are distinguished using the values given in Table 4.19. The numerical results are presented in Figure 4.15 and 542 time steps were calculated. The local times stepping was applied 11 times with a total of 89 small time steps. Here we again used the HLL solver as in [78]. Again, the head and tail velocities

$\tilde{p}$	$\tilde{\rho}$	p_{min}	ρ_{min}
698572.308554 Pa	3.461226 $\frac{\text{kg}}{\text{m}^3}$	0 Pa	903.301343 $\frac{\text{kg}}{\text{m}^3}$

Table 4.19: Maximum vapor pressure and corresponding quantities for the non-linear Tait EOS together with the ideal gas EOS at $T_0 = 437.31057\,\text{K}$



(a) magenta: initial data, red: exact solution, blue: numerical solution; wave structure: shock waves (green) and phase boundaries (red)



(b) Detailed zoom for the pressure; red: exact solution, blue: numerical solution

Figure 4.15: **Solution - Example 6**

of the rarefaction waves are very close to each other, as for example four. In the non-isothermal test case given in [24] the authors obtained the same wave structure. The values in the star region for the pressure are given in Table 4.20. The values for the velocity in the star region are given in Table 4.21. In Figure 4.16 we compare the solution for the pressure for different liquid EOS. The solution structure remains qualitatively the same and the values in the star region are barely distinguishable from another, see Table

	$p_L^{*,-}$	p_V^*	$p_L^{*,+}$
exact	402391.182216 Pa	383546.060043 Pa	402391.182216 Pa
numerical	402391.178337 Pa	383546.056347 Pa	402391.180740 Pa

Table 4.20: Solution Data (Pressure) - Example 6

	$u_L *, -$	u_V^*	$u_L *, +$
exact	$-99.477325\ \frac{\text{m}}{\text{s}}$	$0\ \frac{\text{m}}{\text{s}}$	$99.477325\ \frac{\text{m}}{\text{s}}$
numerical	$-99.477325\ \frac{\text{m}}{\text{s}}$	$0.540292690 \cdot 10^{-6}\ \frac{\text{m}}{\text{s}}$	$99.477325\ \frac{\text{m}}{\text{s}}$

Table 4.21: Solution Data (Velocity) - Example 6

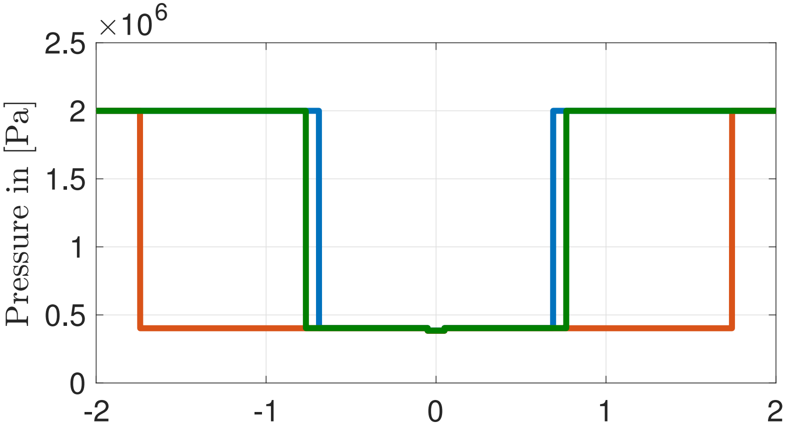


Figure 4.16: **Solution (Pressure) - Example 6:** linear Tait (blue), non-linear Tait (red), stiffened gas (green)

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4.22. The main difference between the three solutions is due to the different sound speeds which affect the rarefaction waves.

	$p_L^{*,-}$	p_V^{*}	$p_L^{*,+}$
linear Tait	403994.450631 Pa	385384.272078 Pa	403994.450631 Pa
non-linear Tait	402391.182216 Pa	383546.060043 Pa	402391.182216 Pa
stiffened gas	403223.628793 Pa	384595.762922 Pa	403223.628793 Pa

Table 4.22: Solution Data (Pressure) for different EOS - Example 6

Part III

Adiabatic Case

Introduction

The third part of this work deals with the case of *non-isothermal* two phase flows. In particular we focus on models that rely on the *adiabatic* (i.e. $q \equiv 0$) Euler equations presented in Section 2.4. Again this topic is related to the work by Hantke et al. [37] for the isothermal case. As mentioned in the second part several questions arise from [37]. In the previous part we already discussed and answered the questions whether a generalization to arbitrary equations of state is possible and how the problem can be treated numerically. Another quite natural question, at least from a mathematical point of view, is if similar results can be obtained in the case of the full Euler system (2.63) - (2.65) [13].

As pointed out before the modeling of such processes is a challenge. The description of the interface between the fluids as well as their interaction is of high complexity. Hence we again focus on the treatment of the interface. We will direct our attention to two phase models that rely on the adiabatic Euler equations and take into account mass transfer between the fluids.
Exemplary we mention the famous models of Baer-Nunziato type. Here both phases are described by their own set of Euler equations. An additional equation for the volume fractions of the phases is considered, see Section 6.3.3. The original model of Baer and Nunziato [3], that does not include the effect of mass exchange between the phases, was modified by Saurel and Abgrall in [71] by introducing relaxation terms for pressures and velocities of the phases. Later in [73] a similar idea allowed the description of phase transition by using relaxation terms for the temperatures and chemical potentials. This idea was picked up for instance by Petitpas et al. in [68] or by Zein et al. in [88].
As in the isothermal case another type of modeling of two phase flows is to use only one set of Euler equations. Each phase has its own equation of state. Phase transitions can be described by a further equation that is called kinetic relation. Again we refer to the well reputed article of Abeyaratne and Knowles [1] that deals with solid-solid interfaces, the papers of Merkle [61] or Hantke et al. [37] on the isothermal Euler equations.
Finally we want to refer to a recent paper of Dumbser et al. [24]. In their work they also consider only one set of equations. Phase transitions take place

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[13] Actually this was the chronological starting point of the whole work. It was supported by the DFG-Grant HA $6471/2-1$, "Eulergleichungen mit Phasenübergängen."

only in thermal equilibrium and no kinetic relation is used. Surprisingly this type of modeling is closely related to the Baer-Nunziato type modeling mentioned above including relaxation terms to describe mass transfer. We come back to this and the above mentioned models later in Section 6.3.3.

The outline of this part is as follows. Chapter 5 discusses the one dimensional adiabatic Euler equations equipped with different assumptions made at the interface. We will discuss the case when no quantities on the interface are present as well as the case when interfacial energy is considered. The main result is that phase transition between the pure phases is not possible when the classical (algebraic) jump conditions are applied. Chapter 5 is an extended version of the published article

[40] M. Hantke and F. Thein. Singular and selfsimilar solutions for Euler equations with phase transitions. *Bulletin of the Brazilian Mathematical Society, New Series*, 47(2):779–786, 2016

The final Chapter 6 gives a nonexistence result for models based on the adiabatic Euler equations. Precisely we will show that condensation by compression and cavitation between pure phases is not possible. The results of Chapter 6 were published in

[39] M. Hantke and F. Thein. Why condensation by compression in pure water vapor cannot occur in an approach based on Euler equations. *Quart. Appl. Math.*, 73(3):575–591, 2015

The most important conclusion, that can be drawn form the results in this part, is that phase transitions between a liquid and a vapor phase are badly described using models based on the adiabatic Euler equations. Thus we strongly recommend to use the isothermal Euler equations discussed in the previous part.

5

Adiabatic Case: Solution Types for Euler Equations with Phase Transitions

5.1 Introduction

In the following we consider Riemann problems for the full system of Euler equations, which was discussed in Section 2.4, applied to liquid-vapor flows. Depending on the assumptions across the phase boundary different kinetic relations can be derived from the second law of thermodynamics. These assumptions influence the structure of the solutions.
The outline is as follows. In Section 5.2 we briefly summarize the considered model and give the jump conditions derived in Section 2.2 for the one dimensional case. The subsequent Section 5.3 treats the case when self-similar solutions are considered. This implies that we obtain the classical jump conditions at the interface. When quantities on the interface are taken into account we obtain singular solutions. This is discussed in Section 5.4. For both cases we discuss the structure of the solution and give an appropriate choice of a kinetic relation.

5.2 Balance Laws and Entropy Inequality

The physical fields are assumed to depend on time $t \in \mathbb{R}_{\geq 0}$ and space $x \in \mathbb{R}$ as before. In regular points of the bulk phases we have the local balances for mass (2.63), momentum (2.64) and energy (2.65)

$$\begin{aligned}\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x}(\rho \mathrm{v}) &= 0,\\ \frac{\partial}{\partial t}(\rho \mathrm{v}) + \frac{\partial}{\partial x}\left(\rho \mathrm{v}^2 + p\right) &= 0,\\ \frac{\partial}{\partial t}\mathcal{E} + \frac{\partial}{\partial x}\left(\mathrm{v}\left(\mathcal{E} + p\right)\right) &= 0.\end{aligned}$$

where $\rho, \mathrm{v}, \mathcal{E}$ denote the *density*, the *velocity* and the *total energy*, respectively. The *specific internal energy* is related to the total energy by $\mathcal{E} = \rho(e + \mathrm{v}^2/2)$, see (2.27). Further the *pressure* p is given by a suited EOS, as discussed in 1.3. Across discontinuities in one dimension the following equations hold, compare (2.19), (2.22) and (2.32),

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{\mathcal{S}} + [\![\rho(\mathrm{v} - W)]\!] = 0, \tag{5.1}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(\rho_{\mathcal{S}} W) + [\![\rho(\mathrm{v} - W)\mathrm{v}]\!] + [\![p]\!] = 0, \tag{5.2}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(e_{\mathcal{S}} + \frac{\rho_{\mathcal{S}}}{2}W^2\right) + \left[\!\!\left[\rho(\mathrm{v} - W)\left(e + \frac{\mathrm{v}^2}{2}\right)\right]\!\!\right] + [\![q + p\mathrm{v}]\!] = 0. \tag{5.3}$$

The *singular mass* and the *singular internal energy* of the discontinuity are denoted by $\rho_{\mathcal{S}}$ and $e_{\mathcal{S}}$. With q we denote the heat flux, for more details see Section 2.2 and the references therein. In the following we always assume, that we have $e_{\mathcal{S}} \equiv 0$ and $\rho_{\mathcal{S}} \equiv 0$ for regular waves propagating through the bulk phase (shock waves, contact discontinuities). In contrast we will consider more general assumptions for phase interfaces. The quantity W is the speed of the discontinuity, which can be a shock, a contact wave or a phase boundary and with $Z = -\rho(\mathrm{v} - W)$ we denote the mass flux. For both quantities we will distinguish between a classical shock wave and the phase boundary (non-classical shock)

$$Z = \begin{cases} Q, & \text{shock wave} \\ z, & \text{phase boundary} \end{cases} \quad \text{and} \quad W = \begin{cases} S, & \text{shock wave} \\ w, & \text{phase boundary} \end{cases}.$$

The mass flux $z = -\rho(\mathrm{v} - w)$ across the phase boundary is in this general situation *not* continuous. It has to be specified by an additional kinetic relation, which has to satisfy the entropy inequality (see also (2.36))

$$\frac{\mathrm{d}}{\mathrm{d}t}s_{\mathcal{S}} + [\![\rho(\mathrm{v} - w)s]\!] + \left[\!\!\left[\frac{q}{T}\right]\!\!\right] = \zeta_{\mathcal{S}} \geq 0\,, \tag{5.4}$$

the *entropy production* ζ_S has to be nonnegative. We consider the singular entropy as a function of the corresponding energy and density, i.e. $s_S = s_S(e_S, \rho_S)$ [1]. The *interface temperature* T_S and the *Gibbs free energy of the interface* g_S are then defined by

$$\frac{1}{T_S} := \frac{\partial s_S}{\partial e_S} \quad \text{and} \quad \frac{g_S}{T_S} := -\frac{\partial s_S}{\partial \rho_S}, \tag{5.5}$$

compare relations (2.43). In the following no heat conduction is taken into account, this means that we have $q \equiv 0$. Assuming that at $t = 0$ the phase boundary is located at $x = 0$ the Riemann initial data may be given by

$$(\rho, \mathrm{v}, p)^T = \begin{cases} (\rho_V, \mathrm{v}_V, p_V)^T & x < 0 \\ (\rho_L, \mathrm{v}_L, p_L)^T & x > 0 \,. \end{cases} \tag{5.6}$$

with V denoting the vapor phase and L the liquid phase, respectively. The Riemann solution can be constructed as discussed in Section 2.4, compare Figure 2.7 and the construction of the solution in Chapter 3. The discussion of rarefaction, shock and contact waves is classical and can also be done as in Section 2.4. Instead we restrict ourselves to the discussion of the phase boundary.

5.3 Self-Similar Solutions

So far we have presented all equations in their most general form, apart from the assumptions made to derive them and the fact that we are concerned with the one dimensional case. In order to construct self-similar solutions we make the following simplifying assumptions at the phase boundary

$$\rho_S \equiv 0 \quad \text{and} \quad e_S \equiv 0 \tag{5.7}$$

to remove the derivative terms in the interface balance equations. This means that the interface has no mass and no energy. As a consequence we have

$$\frac{\mathrm{d}}{\mathrm{d}t} s_S = 0 \,.$$

---

[1] Considering equilibrium thermodynamics with the fundamental equation (1.2) $S = S(E, V)$, this is a quite natural choice.

Moreover the mass flux across the phase boundary is continuous, i.e.

$$[\![\rho(\mathrm{v} - W)]\!] = 0\,.$$

Accordingly the entropy inequality (5.4) becomes

$$-z\,[\![s]\!] = \zeta_{\mathcal{S}} \geq 0\,. \tag{5.8}$$

In view of Remark 2.2.1 this inequality directly implies that the mass flux z is a function of the differences of the specific entropies s of the phases, i.e.

$$z \sim -\,[\![s]\!]\ . \tag{5.9}$$

Thus the mass flux is driven by the difference of the specific entropies of the phases. To derive an explicit kinetic relation we follow the ideas in Dreyer et al. [23], also compare Remark 2.2.1, and make a linear ansatz for the kinetic relation in the following form

$$z = -\tau\,[\![s]\!]\ .$$

The *interface mobility* τ is a positive factor. In [23] τ results from the Maxwell distribution, see also [22], or rather from the classical Hertz-Knudsen theory, see Bond and Struchtrup [10]. With an analogous choice for the mobility we end up with

$$z = -\frac{p_V T_{\mathcal{S}}}{\sqrt{2\pi}}\left(\frac{m}{kT_{\mathcal{S}}}\right)^{\frac{3}{2}}[\![s]\!]\ , \tag{5.10}$$

where k denotes the Boltzmann constant, m the mass of a single molecule of the considered substance and p_V the pressure of the vapor phase. For more details see [23].

Corresponding solutions of the considered Riemann problem consist of five constant states that are separated by four waves see Figure 5.1. The left and the right wave are classical shock or rarefaction waves, that propagate through the bulk phases. In addition the solution has a classical contact wave and a phase boundary, which can be characterized as a non-classical discontinuity. Let us assume the vapor phase is on the left hand side.

For temperatures lower than the critical temperature the specific entropy

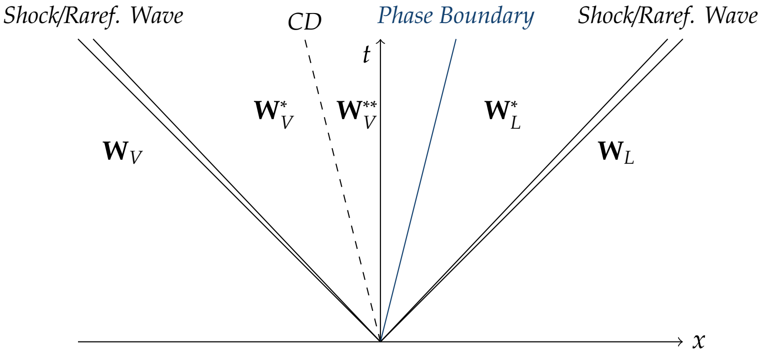

Figure 5.1: Solution structure in the case of (5.7), $\mathbf{W} = (\rho, \rho \mathrm{v}, \mathcal{E})^T$

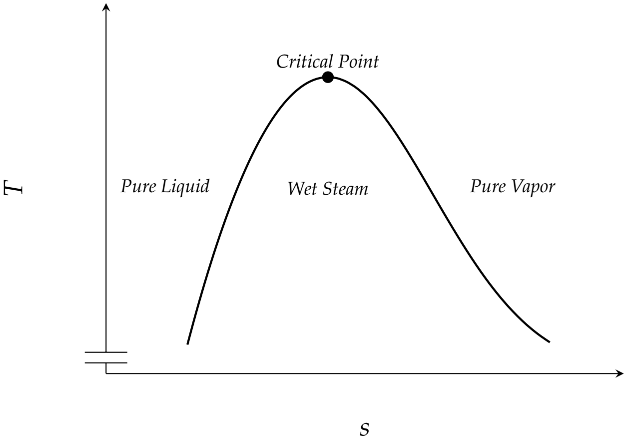

Figure 5.2: Schematic Entropy-Temperature Diagram

of the vapor phase is always larger than the specific entropy of the liquid phase of the same substance, see Figure 5.2. Accordingly we have

$$z \sim -[\![s]\!] > 0\,.$$

This implies that only evaporation processes can take place. In other words, for the simplifying assumptions (5.7) no thermal equilibrium can occur. Further, one can easily obtain that for the above assumption the phase boundary propagates faster than the bulk phases. This implies, that the

contact wave always propagates through the vapor phase.
Additional, even more restrictive, insight can be obtained from the energy balance at the interface [2]. Again, since we have excluded equilibrium we have $(\mathrm{v} - w) = -z/\rho \neq 0$. Using the mass continuity at the interface we obtain for the energy balance at the interface

$$0 = z \left[\!\!\left[e + \frac{p}{\rho} + \frac{1}{2}(\mathrm{v} - w)^2 \right]\!\!\right] \quad \Leftrightarrow \quad 0 = \left[\!\!\left[e + \frac{p}{\rho} \right]\!\!\right] + \frac{1}{2} \left[\!\!\left[\left(\frac{z}{\rho}\right)^2 \right]\!\!\right].$$

Introducing the *specific enthalpy* $h = e + p/\rho$ and using that $\rho_L > \rho_V$ (below the critical point) we yield

$$[\![h]\!] = -\frac{z^2}{2} \left[\!\!\left[\frac{1}{\rho^2} \right]\!\!\right] > 0. \tag{5.11}$$

However, as for the entropy the enthalpy in the (pure) liquid phase is always smaller than the enthalpy in the (pure) vapor phase for temperatures below the critical point [3]. The saturation curves for different variables for water using [84] are exemplary shown in Figure 5.3. Thus we obtain the contradiction

$$0 > [\![h]\!] = -\frac{z^2}{2} \left[\!\!\left[\frac{1}{\rho^2} \right]\!\!\right] > 0. \tag{5.12}$$

Hence it is *not* possible to have a phase boundary between the two (pure) phases in the classical approach that satisfies the jump conditions at the interface. A similar result will also be obtained in the next chapter using different arguments.

Remark 5.3.1. *We want to point out, that the wave structure as well as the non-existence of thermal equilibrium solutions are a direct consequence of the entropy principle (5.8). These phenomena occur for any appropriate choice of a kinetic relation.*

To overcome these phenomena there are two possibilities. On the one hand heat conduction can be taken into account. On the other hand one can weaken the simplifying assumptions (5.7), which leads to singular solutions.

---

[2] This idea was pointed out to me by Christoph Müller and Timon Hitz during our stay in Oberwolfach for the MFO Seminar 1723a.

[3] This can also be obtained by considering the Gibbs free energy in equilibrium $0 = \mathrm{d}g = \mathrm{d}h - T\mathrm{d}s$. This leads to $\mathrm{d}h = T\mathrm{d}s \approx T(s_L - s_V) < 0$.

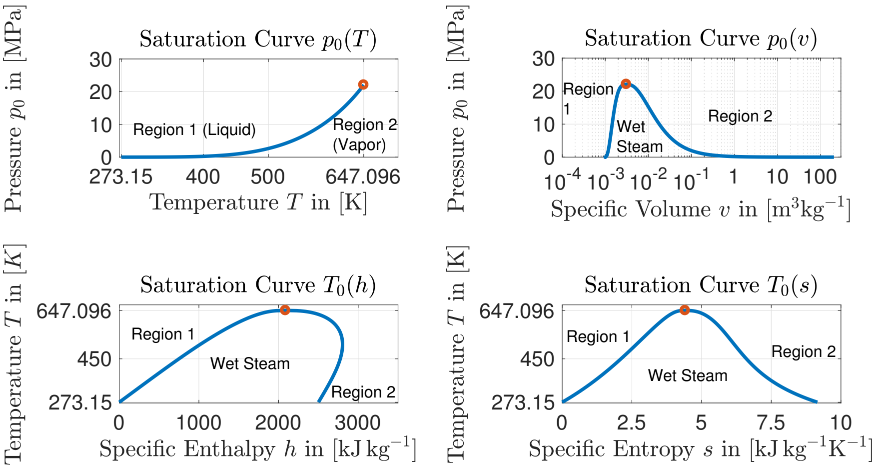

Figure 5.3: The saturation curves for different quantities calculated with the IAPWS-IF97 EOS [84].

5.4 Singular Solutions

As discussed in the previous section we now use weaker simplifying assumptions. As before we neglect the interface density, i.e. $\rho_\mathcal{S} \equiv 0$, but we account for the interface energy. The interface balances for mass and momentum (5.1) and (5.2) reduce to

$$\llbracket \rho(\mathrm{v} - w) \rrbracket = 0, \tag{5.13}$$

$$-z \llbracket \mathrm{v} \rrbracket + \llbracket p \rrbracket = 0, \tag{5.14}$$

Using (5.13) and (5.14) we rewrite (5.3) and obtain the interface energy balance equation

$$\frac{\mathrm{d}}{\mathrm{d}t} e_\mathcal{S} - z \left\llbracket e + \frac{p}{\rho} + \frac{1}{2}(\mathrm{v} - w)^2 \right\rrbracket = 0. \tag{5.15}$$

Using the equations (5.13), (5.14) and (5.15) we can rewrite the entropy inequality (5.4) and yield

$$z \left\llbracket \frac{1}{T_\mathcal{S}} \left(g + \frac{1}{2}(\mathrm{v} - w)^2 \right) + s \left(\frac{T}{T_\mathcal{S}} - 1 \right) \right\rrbracket = \zeta_\mathcal{S} \geq 0\,. \tag{5.16}$$

Equation(5.16) may also easily be derived from equation (2.44) neglecting the heat flux q and assuming a continuous mass flux. Concerning the kinetic relation equation (5.16) implies

$$z \sim \left[\!\!\left[\frac{1}{T_{\mathcal{S}}} \left(g + \frac{1}{2} (\mathrm{v} - w)^2 \right) + s \left(\frac{T}{T_{\mathcal{S}}} - 1 \right) \right]\!\!\right].$$

Due to the derivative in (5.15) the solution of the considered Riemann problem is *not* self-similar. Instead we follow the ideas of Yang [86] and construct solutions in the sense of measures, where a discontinuity appears on the phase interface.

Like Yang we assume a delta-shock, propagating with velocity w and located at $x(t) = w \cdot t$, where the singular value of the interface energy is described by $e_{\mathcal{S}}(t) = e_0 \cdot t$. The solution consists of five constant states, separated by four waves. As before, the right and left waves are classical shock or rarefaction waves. The order of the two middle waves, the contact and the phase boundary, depends on the situation under consideration. With the same arguments as in the previous section we have that in the case of evaporation the contact propagates through the vapor phase and otherwise through the liquid. Accordingly in the case of evaporation we have the same wave structure as before, see Figure 5.1. For the condensation case see Figure 5.4. Note, that in contrast to the solutions of Section 5.3 the interface is now equipped with energy and forms a singularity and hence the solution

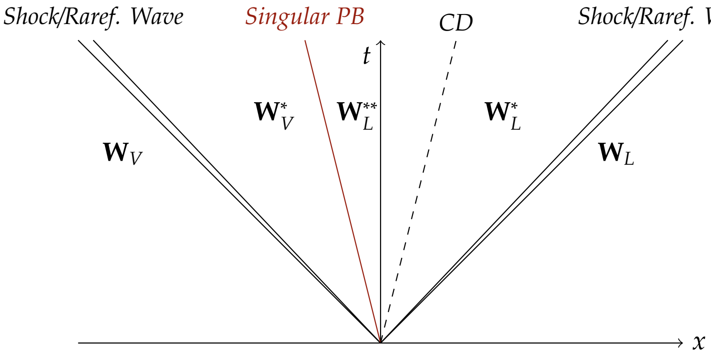

Figure 5.4: Solution structure for the condensation case with a singularity on the phase boundary, $\mathbf{W} = (\rho, \rho \mathrm{v}, \mathcal{E})^T$

is not self-similar anymore.

Assume, the considered solution describes a condensation process, where two shock waves propagate through the bulk phases with velocities S_L and S_R. Further the contact wave propagates with the wave speed S, then the solution at time t is of the following form

$$(\rho, \rho \mathrm{v}, \mathcal{E})^T(t,x) = \begin{cases} (\rho_V, \rho_V \mathrm{v}_V, \mathcal{E}_V)^T, & -\infty < x \leq S_L \cdot t \\ (\rho_V^*, \rho_V^* \mathrm{v}_V^*, \mathcal{E}_V^*)^T, & S_L \cdot t < x < w \cdot t \\ (0, 0, e_0 \delta(x - x(t)) \cdot t)^T, & x = w \cdot t \\ (\rho_L^{**}, \rho_L^{**} \mathrm{v}_L^{**}, \mathcal{E}_L^{**})^T, & w \cdot t < x < S \cdot t \\ (\rho_L^*, \rho_L^* \mathrm{v}_L^*, \mathcal{E}_L^*)^T, & S \cdot t \leq x < S_R \cdot t \\ (\rho_L, \rho_L \mathrm{v}_L, \mathcal{E}_L)^T, & S_R \cdot t \leq x < \infty \end{cases}$$

For solutions with rarefactions or with evaporation states one may find a similar structure.

Analogously to the previous case with the assumptions $\rho_{\mathcal{S}} \equiv 0$ and $e_{\mathcal{S}}(t) = e_0 \cdot t$ one can treat the following two cases

$$\rho_{\mathcal{S}}(t) = \rho_0 \cdot t \quad \text{and} \quad e_{\mathcal{S}} \equiv 0 \tag{5.17}$$

and

$$\rho_{\mathcal{S}}(t) = \rho_0 \cdot t \quad \text{and} \quad e_{\mathcal{S}}(t) = e_0 \cdot t\,. \tag{5.18}$$

In both cases a singularity will form on the phase interface. The structure of the solution is the same as before, but in contrast to the previous case, one obtains singular values for all three components $(\rho, \rho \mathrm{v}, \mathcal{E})^T$. A non-linear ansatz for $\rho_{\mathcal{S}}(t)$ or $e_{\mathcal{S}}(t)$ will lead to more complicated solution structure. In particular the energy of the interface may also be expressed in terms of the temperature of the interface using the equations (1.67) and (1.68)

$$e_{\mathcal{S}} = -T_{\mathcal{S}}^2 \frac{\mathrm{d}}{\mathrm{d}T_{\mathcal{S}}} \left(\frac{\sigma}{T_{\mathcal{S}}} \right) \quad \text{with} \quad \sigma \sim (T_c - T_{\mathcal{S}})^{2\nu}.$$

5.5 Conclusion

Starting from the jump conditions (5.1) - (5.3) we discussed different assumptions that can be made at the interface. First and foremost it is important to note that the heat flux q is not present in the balances for energy and entropy since we consider models relying on the adiabatic Euler equations. In the following we first discussed the case of absent interface quantities which leads to a self-similar solution structure. However, we have shown that (first order) phase transitions between pure phases are not possible due to the difference in the entropies and enthalpies of the phases below the critical point. This leads to the conclusion that we either have to use the heat flux, which is not present here, or account for singular quantities on the interface. In particular we considered the case where the interface is equipped with energy. This results in the loss of the self-similar solution structure.

6 Adiabatic Case: A Nonexistence Result for Two Phase Flows

6.1 Introduction

One can find an extensive literature on cavitating flows, but the opposite question of the creation of a liquid phase by a strong compression is discussed only in rare cases. In the following we consider pure water vapor, that will be highly compressed. This can be realized by a steam filled tube with a flexible piston, see Figure 6.2. If there is no heat exchange with the neighbourhood of the tube, the process is nearly an adiabatic flow. Therefore it can be fairly described by the compressible Euler equations. One may expect, that it is possible to compress the vapor phase such that the vapor will condensate. This means that a liquid phase is created. In fact, it turns out this is impossible in a non-isothermal approach based on Euler equations, which is in agreement with observations from experiments.[1] The main focus of this chapter is to give a mathematical proof for this phenomenon.

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[1] Before writing the article we have inconclusively looked for theoretical results. However, it seemed that there is some kind of common knowledge in certain scientific communities. In particular while writing this thesis we found the following quote in [52], § 132, p. 640: *"[. . .] Kondensationsunstetigkeiten eine selbstständige physikalische Erscheinung sind und nicht das Ergebnis der kompression des Gases in einer gewöhnlichen Stoßwelle. Eine Stoßwelle kann die Dämpfe nicht zur Kondensation bringen, da die Druckerhöhung in einer Stoßwelle eine geringere Auswirkung auf den Übersättigungsgrad hat als die entgegengesetzt wirkende Temperaturerhöhung."* Unfortunately no proof is given, but it strongly underlines the results of the presented nonexistence results (*prove by authority*).

In the case of expanding a liquid under the same boundary conditions, see Figure 6.6, the situation is more complex. Nevertheless, also for the cavitation case we can prove some theoretical results. For detailed discussions of cavitation models we refer to Iben [43] and [44]. This chapter will emphasize the results given in the previous Chapter 5 and further gives alternative arguments.

The chapter is organized as follows. In Section 6.2 we again briefly summarize results for the Riemann Problem for the (adiabatic) compressible Euler equations and the considered equation of state (EOS). The following Section 6.3 deals with compressed water vapor. First we explain the idea for the proof of our statement and then we show for a special choice of equations of state for the phases, that condensation by compression cannot occur. Subsequently we show, that this idea is also applicable to Baer-Nunziato type models with relaxation terms as in Saurel et al. [73] and Zein et al. [88]. Thereafter, we generalize the proof to the *real equation of state for water*. Finally we consider the opposite case of cavitation by expansion in Section 6.5. Some closing remarks are given in Section 6.6.

6.2 Adiabatic Euler Equations

As in the previous chapter the physical fields are assumed to depend on time $t \in \mathbb{R}_{\geq 0}$ and space $x \in \mathbb{R}$. In regular points of the bulk phases we have the local balances for mass, momentum and total energy

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x}(\rho \mathrm{v}) = 0, \tag{6.1}$$

$$\frac{\partial}{\partial t}(\rho \mathrm{v}) + \frac{\partial}{\partial x}\left(\rho \mathrm{v}^2 + p\right) = 0, \tag{6.2}$$

$$\frac{\partial}{\partial t}\mathcal{E} + \frac{\partial}{\partial x}(\mathrm{v}(\mathcal{E} + p)) = 0. \tag{6.3}$$

where $\rho, \mathrm{v}, \mathcal{E}$ denote the *density*, the *velocity* and the *total energy*, respectively. The *specific internal energy* is related to the total energy by $\mathcal{E} = \rho(e + \mathrm{v}^2/2)$, see (2.27). Further the *pressure* p is given by an suited EOS, as discussed in 1.3. Here we consider Riemann problems for the Euler equations, that are given by the above balance equations (6.1)-(6.3), an equation of state and the corresponding *Riemann initial data*

$$(\rho, \mathrm{v}, e)^T = \begin{cases} (\rho_L, \mathrm{v}_L, e_L)^T & x < 0 \\ (\rho_R, \mathrm{v}_R, e_R)^T & x > 0\,. \end{cases} \tag{6.4}$$

As mentioned before this is the simplest choice of initial conditions with piecewise constant data. It is possible and conventional to give initial states for (ρ, v, p) or (p, v, T) instead of initial states for (ρ, v, e). Also other choices are imaginable.

The Riemann problem is very helpful in the context of systems of hyperbolic partial differential equations, because it exhibits all phenomena as shock or rarefaction waves. It is a basic problem in the theory of hyperbolic systems. In numerical methods Riemann problems appear in finite volume methods for systems of conservation laws due to the discreteness of the grid.

For the Riemann problem for the compressible Euler equations equipped with an appropriate equation of state one can construct the exact solution as explained in Section 2.4. The solution is self-similar. It consists of four constant states, that are separated by shock and rarefaction waves and a contact discontinuity. Details can be found in the given literature, e.g. [18, 53, 56, 75, 85].

6.2.1 Definitions and Requirements for the EOS

As mentioned in the previous section we need an EOS to close the system (6.1)-(6.3). Several commonly accepted EOS are available like the van-der-Waals EOS or the Tait EOS, see Section 1.3. As already mentioned a discussion of the adiabatic Euler equations with an arbitrary EOS can be found in [60]. A collective problem is that for any choice of parameters all these equations at the best only locally give a good approximation of the thermodynamic properties of water vapor or liquid water.
On the other hand, the real equation of state for water to the official standard *IAPWS-IF97* based on the standard formulation of Wagner et al. [82, 83, 84] is too complex for analytical consideration. In the following this equation of state is called *real equation of state*.

For the moment we use a modified form of the stiffened gas equation of state, see [73] and also Section 1.3. In particular equation (1.49) and Proposition 1.3.10. Summarized, we have in terms of the pressure and the density

$$e_k(p_k, \rho_k) = \frac{p_k + \gamma_k \pi_k}{\rho_k(\gamma_k - 1)} + q_{e,k}, \tag{6.5}$$

$$T_k(p_k, \rho_k) = \frac{p_k + \pi_k}{C_k \rho_k(\gamma_k - 1)}, \tag{6.6}$$

$$a_k(p_k, \rho_k) = \sqrt{\frac{\gamma_k(p_k + \pi_k)}{\rho_k}}, \tag{6.7}$$

$$s_k(p_k, T_k) = C_k \ln \frac{T_k^{\gamma_k}}{(p_k + \pi_k)^{(\gamma_k - 1)}} + q_{s,k}. \tag{6.8}$$

Here T and s denote the *temperature* and the *specific entropy* of the fluid. The speed of sound is given by a. The index $k = V, L$ indicates the phase under consideration, vapor or liquid. The parameters γ, π, q_e, q_s and C will be specified later. In particular q_e and q_s correspond to the reference values of the energy and entropy e_r and s_r. Note, that for the special choice of $\pi = 0$ and $q_e = 0$ the equation of state reduces to the ideal gas law. The *specific Gibbs free energy* of the phases is given by

$$g_k = e_k + \frac{p_k}{\rho_k} - T_k s_k.$$

As pointed out in Section 1.4 in thermodynamic equilibrium the Gibbs free energies of the phases equal each other and define the coexistence curve in the $T - p$ plane, see Figure 1.1. Now we also want to determine the coexistence curve in the case that both phases are modelled using the stiffened gas EOS with a suited set of parameters. Using the relations (6.5) - (6.8) the Gibbs free energy of each phase can be expressed as a function of the temperature and the pressure. Again if not stated otherwise we denote quantities in a saturation state with a zero index. Now we can obtain the saturation pressure for a given temperature $p_0(T)$ by solving

$$g_L(p_0, T) = g_V(p_0, T). \tag{6.9}$$

Sometimes it is useful to inversely express the temperature as a function of the pressure $T_0(p)$, which can be obtained analogously

$$g_L(p, T_0) = g_V(p, T_0). \tag{6.10}$$

For admissible pressures we obtain the corresponding *saturation temperature*. For the moment we use the same parameters as Saurel et al. [73]. These parameters [2] are given in Table 6.1. For this special choice of parameters

k	γ	π	C	q_e	q_s
vapor	1.43	0	1040	2030000	-23000
liquid	2.35	10^9	1816	-1167000	0

Table 6.1: Parameters for water vapor and liquid water, [73]

we obtain the saturation curve given by the solid line in Figure 6.1. Here

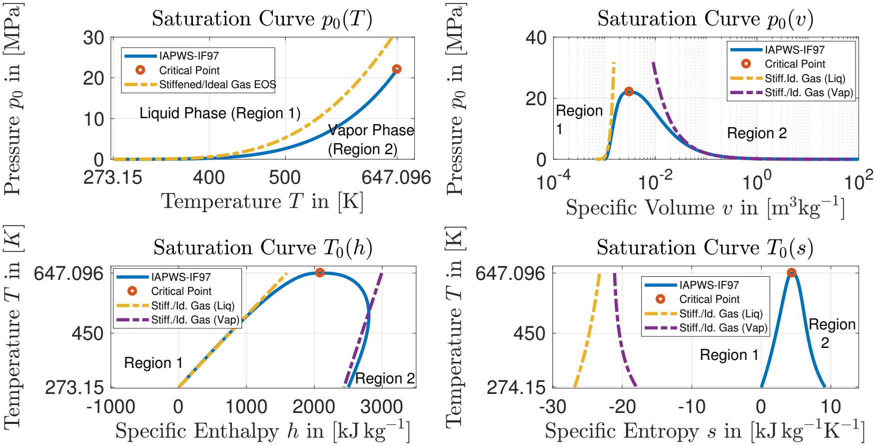

Figure 6.1: Comparison of the saturation curves for different quantities calculated with the IAPWS-IF97 EOS and the stiffened/ideal gas EOS with the parameters given in Table 6.1.

Region 1 belongs to the liquid water phase, whereas Region 2 belongs to the water vapor. The dashed line marks the real saturation line given in [84]. Obviously the precise shape of the saturation line directly depends on the choice for the equations of state and the parameters therein.

Throughout the proof of our statement we will need the Maxwell relations for the Gibbs free energy introduced in Section 1.2, i.e.

$$\left(\frac{\partial g}{\partial T}\right)_p = -s \quad \text{and} \quad \left(\frac{\partial g}{\partial p}\right)_T = \frac{1}{\rho}. \tag{6.11}$$

---

[2] We have $[\pi] = \mathrm{Pa}$, $[C] = \mathrm{Jkg}^{-1}\mathrm{K}^{-1}$, $[q_e] = \mathrm{Jkg}^{-1}$, $[q_s] = \mathrm{Jkg}^{-1}\mathrm{K}^{-1}$.

6.3 Condensation by Compression

6.3.1 Wave Curve in the $p - T$ Phase Space

First we consider the case of the compression of water vapor. This case can be simulated by a tube which is filled with vapor and equipped with a flexible piston, which is highly sped up to compress the vapor phase, see Figure 6.2. The compression of water vapor will lead to an increase of the pressure and the density of the vapor phase. From the theory of the Euler equations we know, that a shock wave will propagate through the vapor phase. Assume that the state ahead of the shock is given by $(\hat{\rho}, \hat{\mathrm{v}}, \hat{p})$. The state behind the shock is denoted by $(\rho^*, \mathrm{v}^*, p^*)$. The jump conditions (2.66) - (2.68)

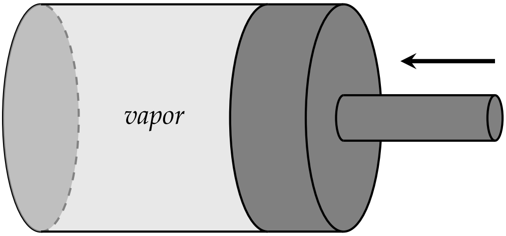

Figure 6.2: Compression of water vapor

$$\begin{aligned} [\![\rho(\mathrm{v} - S)]\!] &= 0, \\ \rho(\mathrm{v} - S)\,[\![\mathrm{v}]\!] + [\![p]\!] &= 0, \\ \left[\!\!\left[e + \frac{p}{\rho} + \frac{1}{2}(\mathrm{v} - S)^2 \right]\!\!\right] &= 0. \end{aligned}$$

and equation (6.5) can be combined to obtain

$$\frac{\rho^*}{\hat{\rho}} = \frac{\left(\frac{p^*}{\hat{p}}\right) + \left(\frac{\gamma - 1}{\gamma + 1}\right) + \frac{2\gamma\pi}{\hat{p}(\gamma + 1)}}{\left(\frac{\gamma - 1}{\gamma + 1}\right)\left(\frac{p^*}{\hat{p}}\right) + 1 + \frac{2\gamma\pi}{\hat{p}(\gamma + 1)}}. \tag{6.12}$$

For details of the derivation of relation (6.12) we exemplary recommend the book of Toro [78]. Again we emphasize, that this relation holds only for the generalized stiffened gas law (6.5) - (6.8). Using the equation of state (6.6) we easily obtain an analogous relation for the pressure and the temperature, which is given by

$$\frac{\hat{T}}{T^*} = \frac{\hat{p} + \pi}{p^* + \pi} \cdot \frac{p^*(\gamma + 1) + \hat{p}(\gamma - 1) + 2\gamma\pi}{\hat{p}(\gamma + 1) + p^*(\gamma - 1) + 2\gamma\pi \dfrac{\hat{p}}{p^*}}. \tag{6.13}$$

From Equation (6.13) we obtain the wave curve $T^*(p^*; \hat{p}, \hat{T})$ in the (p, T)-phase space. With this curve we can describe all states (p^*, T^*) that can be connected to the initial state $(\hat{p}, \hat{T})$ by a shock wave.

Now assume that the vapor phase with initial pressure and temperature $(\hat{p}, \hat{T})$ is compressed sufficiently strong such that a liquid phase is created, then the corresponding wave curve $T^*(p^*; \hat{p}, \hat{T})$ must have an intersection point with the saturation line, see the sketch in Figure 6.3. We want to prove that this is impossible. For the proof we assume the existence of the intersection point and derive a contradiction.

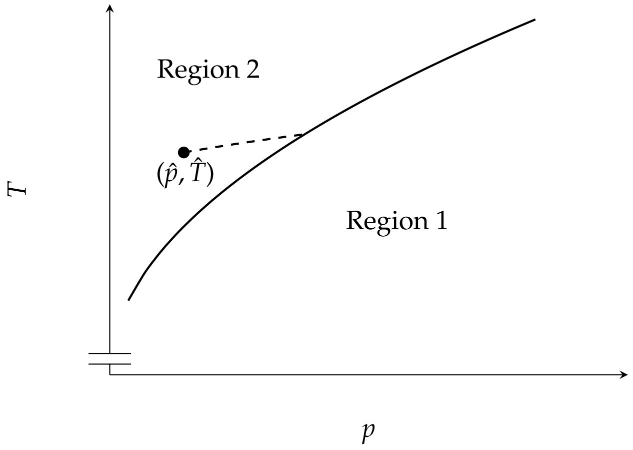

Figure 6.3: Solid line: saturation curve $T_0(p)$, dashed line: wave curve with initial state

6.3.2 Proof of the Statement for a Particular EOS

Let us denote the intersection point of the wave curve and the saturation line by (p^*, T^*). Then the function

$$\hat{T}(\hat{p}; p^*, T^*) = T^* \cdot \frac{\hat{p}}{p^*} \cdot \frac{p^*(\gamma_V + 1) + \hat{p}(\gamma_V - 1)}{\hat{p}(\gamma_V + 1) + p^*(\gamma_V - 1)} \tag{6.14}$$

denotes all admissible initial states $(\hat{p}, \hat{T})$. Here we already used the fact that for the vapor phase we have $\pi = 0$. Let the prime $'$ denote the derivative of the temperature functions with respect to the pressure. At the intersection point the following relation must hold

$$\hat{T}'(p^*) \leq T_0'(p^*). \tag{6.15}$$

By a simple calculation we find

$$\hat{T}'(p^*; p^*, T^*) = \frac{T^*}{p^*} \cdot \frac{\gamma_V - 1}{\gamma_V}. \tag{6.16}$$

To find $T_0'(p^*)$ we start with the equilibrium condition (6.10) and express the Gibbs free energies of the phases as functions of p and T. We yield

$$g_k(p, T) = C_k T \gamma_k + q_{e,k} - C_k T \ln \frac{T^{\gamma_k}}{(p + \pi_k)^{\gamma_k - 1}} - T q_{s,k}$$

with $k = L, V$. Using the implicit function theorem and

$$f(p, T_0) = g_V(p, T_0(p)) - g_L(p, T_0(p)) = 0 \tag{6.17}$$

we derive

$$\begin{aligned}
\frac{\partial f}{\partial p} &= C_V(\gamma_V - 1)\frac{T_0}{p} - C_L(\gamma_L - 1)\frac{T_0}{p + \pi_L} \\
\frac{\partial f}{\partial T_0} &= -C_V \ln \frac{T_0^{\gamma_V}}{(p)^{\gamma_V - 1}} - q_{s,V} + C_L \ln \frac{T_0^{\gamma_L}}{(p + \pi_L)^{\gamma_L - 1}} \\
&= C_L\gamma_L - C_V\gamma_V + \frac{q_L - q_V}{T_0}
\end{aligned}$$

and finally

$$T_0'(p^*; T^*) = T^* \cdot \frac{\dfrac{C_V(\gamma_V - 1)}{p^*} - \dfrac{C_L(\gamma_L - 1)}{p^* + \pi_L}}{C_V\gamma_V - C_L\gamma_L + \dfrac{q_{e,V} - q_{e,L}}{T^*}} < T^* \cdot \frac{\dfrac{C_V(\gamma_V - 1)}{p^*}}{C_V\gamma_V}. \tag{6.18}$$

This is clear because

$$-\frac{C_L(\gamma_L - 1)}{p^* + \pi_L} < 0 \quad \text{and} \quad 0 < -C_L\gamma_L + \frac{q_{e,V} - q_{e,L}}{T^*}.$$

Obviously (6.18) implies

$$T_0'(p^*; T^*) < \frac{T^*}{p^*} \cdot \frac{\gamma_V - 1}{\gamma_V} = \hat{T}'(p^*; p^*, T^*). \tag{6.19}$$

This is a contradiction, see (6.15). Accordingly we have

Theorem 6.3.1. *Using the equations of state (6.5) - (6.8) and the parameters given in Table 6.1 condensation by compression of pure water vapor cannot occur.*

6.3.3 Short Discussion of Different Phase Transition Models

In the following paragraph we explain, why the proof of our statement given in Subsection 6.3.2 resp. in Subsection 6.4 is applicable for all considered models based on Euler equations.

The pure water vapor phase can be described by a single set of Euler equations. The compression leads to an increase of the density and the pressure as already mentioned in the previous section. One may assume that for sufficiently strong compression the vapor phase starts to condensate. This means, that a liquid phase is created. Of course, for any state (p, T) which is in the interior of Region 2 (water vapor), the vapor phase is situated in a stable state. In order that condensation can happen, there must be a mechanism for phase transition. Therefore, it is clear that in the case of condensation the wave curve must have an intersection point with the saturation line. For this it does not matter, whether phase transition is modeled by a kinetic relation as in [37, 61] or by using an equilibrium assumption as done in [24].

Using a kinetic relation, a nucleation criterion is used, see Chapter 3 and [37]. Here a critical state is reached, in which the vapor phase starts to condensate, which implies the intersection point.

In the work by Dumbser et al. [24] phase transition is modeled by an equilibrium assumption. For any given temperature T and $p < p_0(T)$ the pair (T, p) describes some vapor state. Analogously (T, p) with $p > p_0(T)$ describes the fluid in the liquid state. For $p = p_0(T)$ one may have water vapor or liquid water as well as a mixture of both fluids. The fluid at the saturation state is defined by its temperature and the mass fraction or equivalently by its

pressure and the mass fraction of the vapor/liquid phase. All corresponding states in the $p - T$ phase plane are located at the saturation line. For more details see Iben et al. [45]. Nevertheless, for condensation a wave curve must have an intersection point with the saturation line.
The Euler equations are only valid for pure fluids or homogeneous mixtures in the thermodynamic equilibrium. For models that use only one set of Euler equations, as discussed before, only pure fluids are present. On the other hand in the literature often models of Baer-Nunziato type are used to describe the considered situation. The generalized Baer-Nunziato model is given by a two phase model using two sets of Euler equations

$$\begin{aligned}
\frac{\partial}{\partial t}\alpha_k\rho_k + \frac{\partial}{\partial x}\alpha_k\rho_k \mathrm{v}_k &= \pm\dot{m} \\
\frac{\partial}{\partial t}\alpha_k\rho_k \mathrm{v}_k + \frac{\partial}{\partial x}\alpha_k\left(\rho_k \mathrm{v}_k^2 + p_k\right) &= \pm P\frac{\partial}{\partial x}\alpha_k \pm M \\
\frac{\partial}{\partial t}\alpha_k\rho_k\left(e_k + \frac{1}{2}\mathrm{v}_k^2\right) + \frac{\partial}{\partial x}\left[\rho_k\left(e_k + \frac{1}{2}\mathrm{v}_k^2\right) + p_k\right]\mathrm{v}_k &= \mp P\frac{\partial}{\partial t}\alpha_k \pm E
\end{aligned}$$

$k = 1, 2$ and a further equation to describe the volume fractions of the phases

$$\frac{\partial}{\partial t}\alpha_1 + U\frac{\partial}{\partial x}\alpha_1 = A$$

with the same notations as before. Further, α_k denotes the volume fraction of phase k. The sources $A, \dot{m}, M, E$ on the right hand side of the equations describe the exchange of mass, momentum and energy. They include relaxation terms for velocity, pressure, temperature and Gibbs free energy of the phases, that guarantee, that both phases relax to thermodynamic equilibrium. The pressure P and the velocity U have to be defined by some closure law, see [71, 73] or [88].
Again we start with a pure vapor phase, that will be compressed. For numerical reasons the volume fraction of the pure phase is assumed to be $1 - \varepsilon$, whereas the volume fraction of the absent phase is assumed to be ε. Typically one uses $\varepsilon = 10^{-8}$, see for instance Saurel and Abgrall [71].
Mass transfer is described by the Gibbs free energy relaxation term. Condensation will occur only in the case, that the specific Gibbs free energy of the vapor phase is larger than the specific Gibbs free energy of the (artificial) liquid phase. This is not the case for any set of initial data that describes a pure water vapor phase. Therefore there is no contribution by the relaxation terms as long as (T, p) is in the interior of Region 2 (vapor phase).

In regions of constant volume fractions the system decouples. The solution for each phase can be determined separately. This implies that the relations of the single phase Euler equations are also valid for the Baer-Nunziato model in the present case. In order that condensation can occur the vapor phase must be compressed in such a manner, that the specific Gibbs free energy of the vapor phase is larger than the specific Gibbs free energy of the (artificial) liquid phase. This implies an intersection point of the wave curve with the saturation line.

6.4 Extension to the Real EOS for Water

In the previous Section 6.3.2 we have proved, that condensation by compression can not occur for the chosen equations of state with parameters given in Table 6.1. On the other hand, in Figure 6.1 we can see, that this choice gives a very bad approximation of the real saturation curve for higher temperatures. We now generalize our statement using the results from the last section. We want to show, that for the *real equation of state* and for *good* approximations of the real equation of state condensation by compression cannot occur. The proof uses the same arguments as before.

We start with an arbitrary initial state in the vapor region and we consider the corresponding wave curve. Assume, (p^*, T^*) is the intersection point of the curve $\hat{T}(\hat{p}; p^*, T^*)$ of all admissible initial states in the $p-T$ phase space with the real saturation line $T_0(p)$. We compare the derivatives and find the contradiction.

6.4.1 Approximation of the Real EOS

For our purpose it is sufficient to find a good approximation of the real equation of state in a small neighborhood of the saturation line. In the following we show how to find suitable parameters, coming from the intersection point (p^*, T^*). This is an improvement of the method of Le Metayer et al. [63], which is a modification of the idea introduced by Barberon and Helluy [4].

Vapor Phase

For any temperature T^* the corresponding (real) saturation pressure is known by the real formulas given by Wagner [82, 83]. The same is true for the corresponding vapor density ρ_V^*, the speed of sound a_V^*, the entropy s_V^* and the internal energy e_V^*. For simplicity we choose $\pi_V = 0$. Then from (6.7) we directly obtain γ_V. Next we calculate $q_{e,V}$ from (6.5), C_V from (6.6) and $q_{s,V}$ from (6.8). The results are given in Figure 6.4.

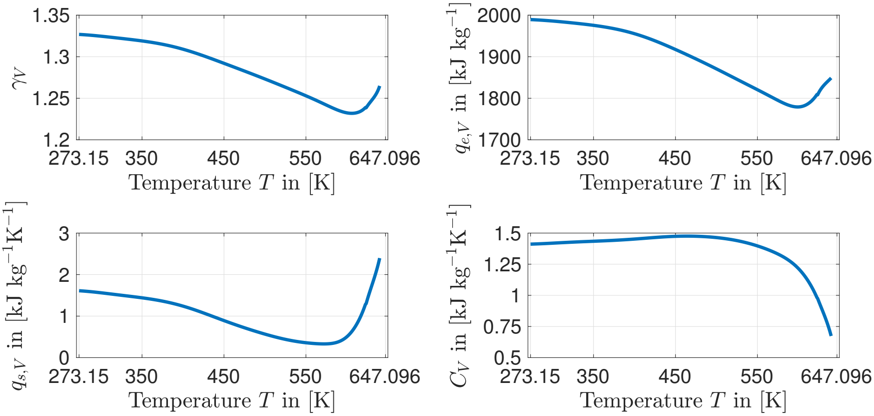

Figure 6.4: Local optimal parameters for the vapor phase

Liquid Phase

For the liquid phase we disclaim the simplifying assumption for the parameter π. Accordingly we are looking for five parameters. Thus, beside the relations (6.5) - (6.8), we can use a further relation. Therefore we consider the specific heat capacity at constant pressure which is given by

$$T\left(\frac{\partial s}{\partial T}\right)_p = C_p,$$

see Definition 1.3.1 (ii). Using (6.5), (6.6) and (6.8) we find that

$$\begin{aligned} C_{p,L} &= T_L \frac{\partial s_L(T_L, p_L)}{\partial T_L} = C_L \gamma_L \\ &= \frac{1}{T_L}\left(\frac{p_L + \gamma_L \pi_L}{\rho_L(\gamma_L - 1)} + \frac{\gamma_L p_L - p_L}{\rho_L(\gamma_L - 1)}\right) \\ &= \frac{1}{T_L}\left(e_L - q_{e,L} + \frac{p_L}{\rho_L}\right). \end{aligned}$$

This gives us the further relation

$$e_L = C_{p,L}T - \frac{p_L}{\rho_L} + q_{e,L}, \tag{6.20}$$

where $C_{p,L}$ denotes the specific heat capacity at constant pressure of the liquid phase. Again we use the real equation of state to obtain the liquid density ρ_L^*, the speed of sound a_L^*, the entropy s_L^*, the internal energy e_L^* as well as the specific heat capacity $C_{p,L}^*$. Then from (6.20) we find $q_{e,L}$. After that we calculate π_L and γ_L from (6.5) and (6.7). Finally we obtain C_L from equation (6.6) and $q_{s,L}$ from equation (6.8). The results are given in Figure 6.5. Using the parameters $\pi_V, \pi_L, \gamma_V, \gamma_L, C_V, C_L, q_{e,V}, q_{e,L}, q_{s,V}, q_{s,L}$ obtained in this section, the equations of state (6.5) - (6.8) give the exact values for the densities, the internal energies, the entropies and the sound speeds at

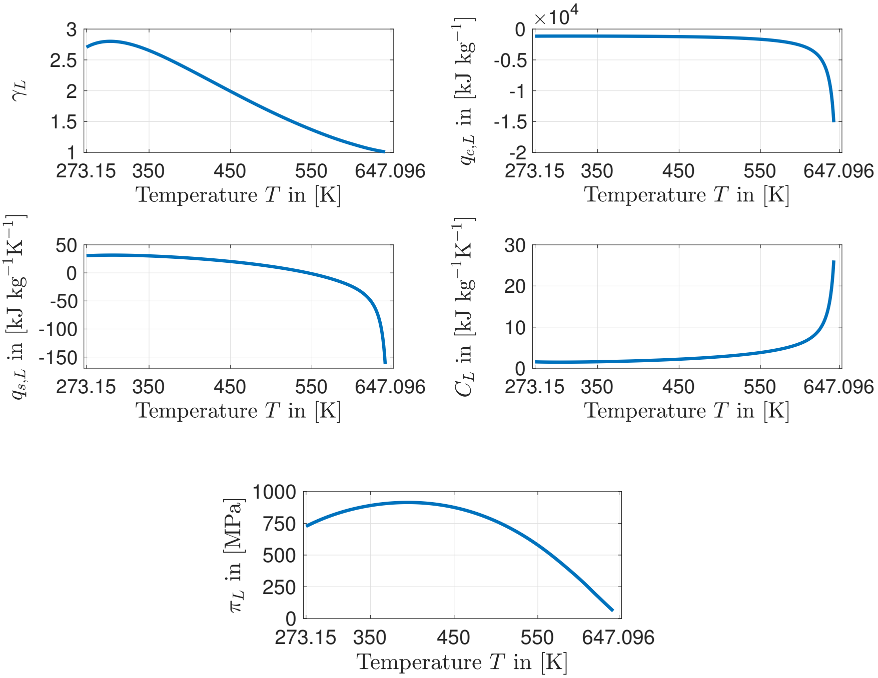

Figure 6.5: Local optimal parameters for the liquid phase

saturation state (p^*, T^*). Also we obtain the exact values for the Gibbs free energies and the enthalpies. From the Maxwell relations (6.11) as well as equation (6.17) and the implicit function theorem we see, that we also find the exact value

$$T_0'(p^*; T^*).$$

Due to the smoothness of all expressions for any given tolerance $\varepsilon > 0$ we find a sufficiently small neighborhood of the saturation state (p^*, T^*) such that all relevant physical states $\rho_k, e_k, s_k, a_k, g_k$ are approximated with a deviation less then ε.

6.4.2 Proof of the Statement for the Real EOS

Assume, for any initial state in the vapor region sufficiently close to the saturation line, the corresponding wave curve in the $p - T$ phase space and the (real) saturation line have the intersection point (p^*, T^*). Assume further, that we used the optimal parameters $\pi_V, \pi_L, \gamma_V, \gamma_L, C_V, C_L, q_{e,V}, q_{e,L}, q_{s,V}, q_{s,L}$, such that the equations of state (6.5) - (6.8) give the exact values for $\rho_k, e_k, s_k, a_k, g_k$ for both phases at saturation state (p^*, T^*). Then the following relation must hold at the intersection point

$$\hat{T}'(p^*) \leq T_0'(p^*). \tag{6.21}$$

As before $\hat{T}(\hat{p}; p^*, T^*)$ denotes all admissible initial states $(\hat{p}, \hat{T})$ in the vapor region, in a sufficiently small neighborhood of (p^*, T^*). For the derivative we have

$$\hat{T}'(p^*; p^*, T^*) = \frac{T^*}{p^*} \cdot \frac{\gamma_V - 1}{\gamma_V}. \tag{6.22}$$

Moreover, we have

$$T_0'(p^*; T^*) = T^* \cdot \frac{\dfrac{C_V(\gamma_V - 1)}{p^*} - \dfrac{C_L(\gamma_L - 1)}{p^* + \pi_L}}{C_V\gamma_V - C_L\gamma_L + \dfrac{q_{e,V} - q_{e,L}}{T^*}}. \tag{6.23}$$

In both equations (6.22) and (6.23) we used the local optimal parameters. As already explained at the end of Section 6.4.1, equation (6.23) gives the exact value for the derivative. Simple estimations show, that

$$\hat{T}'(p^*) > T_0'(p^*). \tag{6.24}$$

Accordingly, there is no such intersection point. Due to the smoothness of all expressions and the exactness of (6.23) this statement is true for the real equation of state and for all sufficiently good approximations of the real equation of state. If there is any set of parameters $\pi_V, \pi_L, \gamma_V, \gamma_L, C_V, C_L, q_{e,V}, q_{e,L}, q_{s,V}, q_{s,L}$ such that (6.24) is not satisfied, then the parameters obviously give a coarse approximation of the saturation line and the result is not meaningful. The same is true for any other choice of equations of state for the liquid and the vapor phase. We summarize

Theorem 6.4.1. *Using the real equations of state [84] or any good approximation of the real equation of state nucleation by compression cannot occur.*

6.5 Cavitation by Expansion

After the discussion of condensation by compression one may ask for the opposite case of cavitation by expansion. We will see, that this process is more complicated and we will distinguish between two cases. The liquid phase will be expanded in a manner that phase transition will occur. This case corresponds to a cavitation tube, which is a tube filled with liquid water and a flexible piston, see Figure 6.6. To illustrate the physics we give the $s-T$ diagram in Figure 6.7, where the path (1) corresponds to the process considered. We have seen, that the Baer-Nunziato type relaxation model allows the coexistence of both the vapor and the liquid phase in the same point of the physical domain at the saturation state. The same is true for the Eulerian model used by Dumbser et al. [24]. Here the phase transition is modeled assuming equilibrium. The mixture is called *wet steam*. An expansion process such that a mixture of water vapor and liquid water (wet

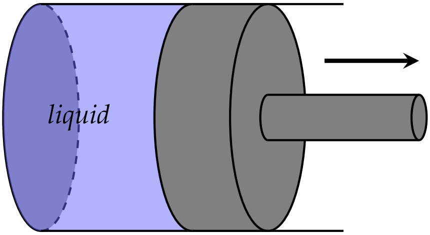

Figure 6.6: Expansion of liquid water

steam) is created, we call the process *weak cavitation*. On the other hand, if pure water vapor is created, we call this process *strong cavitation*.

6.5.1 Cavitation in the Weak Sense

If the liquid phase is expanded, a rarefaction wave will propagate through the liquid phase. In analogy to the condensation case we start with an arbitrary set of initial data in the liquid phase (Region 1). We construct the wave curve, that connects the initial state to all possible states behind the rarefaction wave. If (weak) cavitation, by sufficiently strong expansion, can occur this wave curve must have an intersection point with the saturation line. It is not surprising, that this is usually the case. Numerous examples can be found in the literature, see for instance the example *cavitation by strong rarefaction* using one set of Euler equations and the equilibrium assumption in Dumbser et al. [24]. See further the *expansion tube problem* in Zein et al. [88] using the Baer-Nunziato type relaxation model.

6.5.2 Cavitation in the Strong Sense

For the moment we restrict ourselves to the two model types, that allow the coexistence of vapor and liquid, as in [24, 88]. Models, using a kinetic

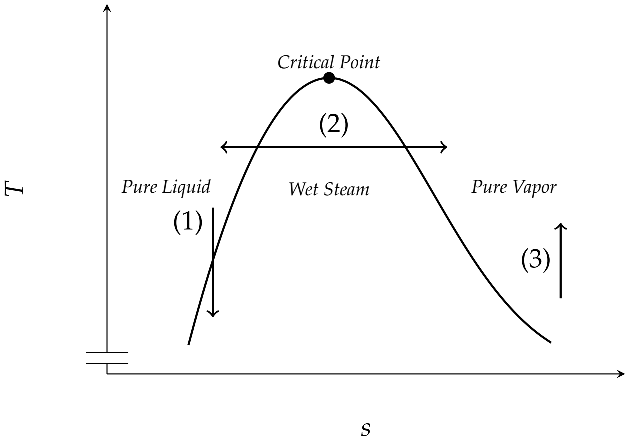

Figure 6.7: Schematic Entropy-Temperature Diagram with different processes: (1) isentropic expansion - rarefaction wave, (2) isothermal path, (3) isentropic compression, see Iben [43]

relation will be discussed later.

One may assume that for sufficiently strong expansions one may create pure water vapor. To illustrate that situation we refer to Figure 6.8. As pointed out in Section 1.4 the saturation states in the $T-p$ phase plane are located on a single curve, whereas the coexistence curve in the $p-\rho$ phase plane will enclose a whole domain of saturation states due to the jump in the volume, compare Figures 1.1 and 1.2. The wet steam region is bounded by the saturation (solid) lines. Assume, there is any initial liquid state, marked by the star and assume further, the liquid is expanded in a manner that pure water vapor is created. This state is indicated by the circle. Then there is a rarefaction wave curve, connecting the star and the circle state. This wave curve crosses the two curves $\rho_k(p_0)$. The same situation in the $p-T$ phase plane is given in Figure 6.9. In the following we will show, that strong cavitation for the models considered cannot occur. The argument is similar to the argument in the condensation case. Assume, the circle state exists. This implies the existence of a rarefaction wave curve that connects both the circle and the star state. The intersection point of the wave curve and the saturation curve $T_0(p)$ in the $p-T$ phase plane is called (p^*, T^*). Let us consider that part of the wave curve, that is located in the vapor in Region 2. We denote this curve by $\hat{T}(p; p^*, T^*)$. As before for the intersection point

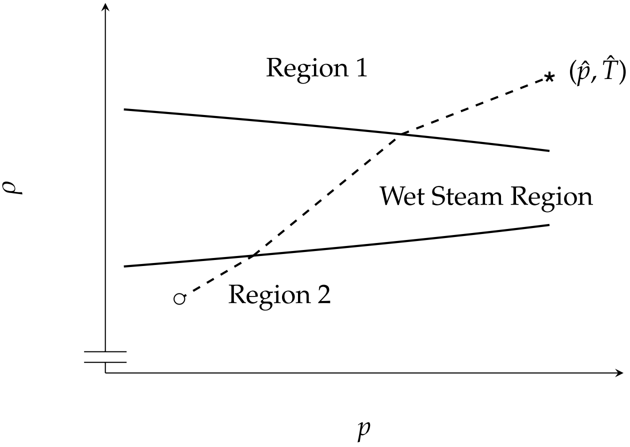

Figure 6.8: Solid line: saturation curves $\rho_V(p_0)$, $\rho_L(p_0)$, dashed line: wave curve with initial state and final pure water vapor state

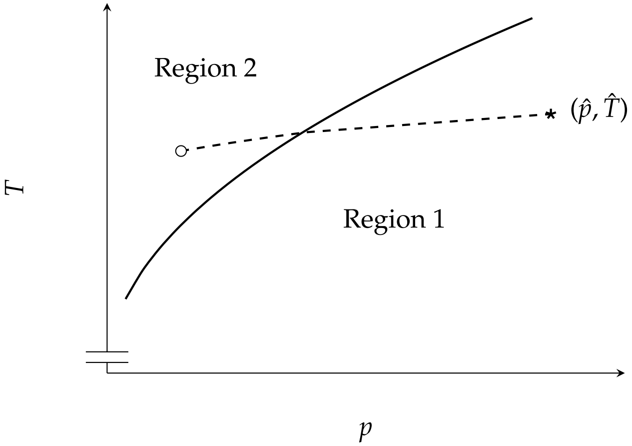

Figure 6.9: Solid line: saturation curve, dashed line: wave curve, star: initial state, circle: pure water vapor state

we must have

$$\hat{T}'(p^*; p^*, T^*) \leq T_0'(p^*).$$

The wave curve is found to be

$$\hat{T}(p; p^*, T^*) = T^* \left(\frac{p}{p^*}\right)^{\frac{\gamma_V - 1}{\gamma_V}}. \tag{6.25}$$

This directly follows from Equation (6.8) and the fact, that the entropy is constant across a rarefaction wave. Equation (6.25) implies

$$\hat{T}'(p^*; p^*, T^*) = \frac{T^*}{p^*} \cdot \frac{\gamma_V - 1}{\gamma_V}. \tag{6.26}$$

This gives a contradiction, see (6.22) and (6.23).

Theorem 6.5.1. *Using the real equation of state or any good approximation of the real equation of state strong cavitation by expansion cannot occur in an approach based on Euler equations and an equilibrium assumption, [24, 88].*

There is an alternative, very simple argument to show, that a pure liquid state and a pure water vapor state cannot be connected by a rarefaction wave.

As already mentioned it is a well known fact, that the entropy is constant across a rarefaction wave. However, as already noted in the previous Section 5.3, we have that for any temperature between triple point temperature and critical temperature $T_{tripel} = 273.16$ K $< T < T_{crit} = 647.096$ K the entropies satisfy the inequalities

$$s_L < s_{crit} < s_V. \tag{6.27}$$

Obviously there are no (pure) liquid and (pure) vapor states with the same entropy. This also can be seen in Figure 6.7.

Using an Eulerian approach like Dumbser et al. [24] one can obtain only weak cavitation. Wet steam is created, which is a mixture of water vapor and liquid water at saturation state. For the entropy one has

$$s_{mix} = \mu s_V + (1 - \mu) s_L \tag{6.28}$$

where $\mu \in [0, 1]$ denotes the vapor mass fraction, see [24]. Due to Equation (6.27) the value μ is bounded for cavitation starting from pure liquid water. Using the steam tables of Wagner [83] we find

$$\mu \leq 0.5. \tag{6.29}$$

In contrast to the equilibrium models discussed in the first part of Section 6.5.2 models using a kinetic relation are able to produce strong cavitation. This is clear by Section 6.5.1. A rarefaction wave curve in the liquid Region 1 can have an intersection point with the saturation line. Here a critical state is reached. A cavitation criterion can be used, see Chapter 3 or Hantke et al. [37]. The liquid phase starts to evaporate and a pure vapor phase is created. An important difference to the previous models is, that the solution is not smooth and entropy production by phase transition is allowed. Therefore there is no contradiction to previous results.

6.6 Conclusions

We have seen, that condensation by compression cannot occur in an Eulerian approach. Due to the compression of the water vapor not only the pressure but also the temperature is increasing. Due to the rising temperature the saturation pressure is increasing. The key point is, that the saturation pressure increases much faster than the pressure inside the vapor phase. Therefore phase transition cannot take place. From observations of nearly adiabatic flows, see Figure 6.6 and 6.2 this phenomenon is known.

- The Euler equations correctly reflect this behavior. We presented a mathematical proof for this.

- Adiabatic compression of vapor does not lead to a liquid phase, see Figure 6.7, path (1). To reach this state, a negative heat flow has to be used. This is equivalent to the use of isothermal Euler equations such as presented in Chapter 3. This corresponds to path (1) in Figure 6.7.

This effect comes up in much weaker form in the case of cavitation. The reason may be that the temperature changes due to the expansion are much smaller.

- It is not possible to evaporate a pure liquid by a rarefaction wave completely, only with external supply of energy, see again Figure 6.7. This is also equivalent to the use of isothermal Euler equations, see Figure 6.7, path (2).

- We gave a mathematical proof for this.

On the other hand this shows, that heat flow plays an important role in cavitation processes or in condensation processes caused by compression. Thus Eulerian models (i.e. without heat transfer) are not appropriate to describe such effects.

7 Open Questions

In this chapter we want to summarize several questions or problems that arise in the context of this work. Some of them might be rather easy whereas other questions may be more difficult to answer. However, the decision whether a question is easy to answer or not is definitely something that is difficult to answer in advance. A presumably easy problem may hide severe difficulties and with the right idea a difficult problem may be solved in an instant.

The stated problems are *not* ordered by priority. We try to sort them according to the previous content.

Problem 1. The mathematical problems and results related to this work are an interesting topic on their own and their treatment is already justified by mathematical interest. However, since the studied models are used in several applications the obtained results should be compared with real world experiments. We found it difficult to get different experimental data (e.g. for two phase flows) that are suited to serve for a comparison with the numerical simulations. Hence we think that mathematicians, physicists and engineers working on this field should set up a series of test problems that then should be performed in experiments such that the results may be used to validate different approaches.

Problem 2. It is a well known result, that for that the entropy jump of weak shock wave is of third order in the strength of the shock, see [9, 18, 60]. Now the question arises how this result is changed when the generalized jump conditions are used? For example what are the consequences for the entropy jump when the energy of the interface is considered?

Problem 3. To obtain the general existence result in Chapter 3 we assumed that $\mathcal{G} > 0$ in both phases. Does a similar result hold for the case of $\mathcal{G} < 0$? Regarding the possible applications it should be sufficient to exclusively discuss this case for the vapor phase. Further we think that this should only affect the solution of the Riemann problem. Theorem 3.2.2 should remain valid for $\mathcal{G}_V < 0$. For single phases the case of a nonconvex EOS is discussed in [67].

Problem 4. The kinetic relation in Chapter 3 was obtained by assuming that the mass flux is directly proportional to the jump of $g + e_{kin}$. Which properties should a kinetic relation of the form $z = f([\![g + e_{kin}]\!])$ fulfill in order to obtain similar results? See also Remark 2.2.1.

Problem 5. So far we included the case that a phase may be created. The description of the opposite case (e.g. a completely evaporating droplet) would also be nice to know.

Problem 6. The results of Chapter 3 are obtained under certain assumptions. These assumptions are sufficient to state these results. Do these assumptions already cover all relevant EOS? Is it possible to drop some of the (technical) assumptions?

Problem 7. As for most one dimensional problems it would be desirable to extend the discussion to the two and three dimensional case. This would imply to consider surface tension.

Problem 8. We proposed an approach to solve one dimensional Riemann problems for two phase flows including nucleation and cavitation. As previously mentioned there are promising results for two dimensions which currently are not able to treat phase creation. This is a major issue which is directly connected to the analytical discussion. Especially the treatment of the curvature in the numerical method is a major issue.

Problem 9. Is there a reliable and fast direct solver for the two phase Riemann problem[1]?

Problem 10. In the third part of this work we have shown that it is necessary to consider interface quantities in the adiabatic case. This case of singular solutions has to be properly discussed. However, we think that in the case of two phsae flows with phase transition the need for interface quantities in the adiabatic case just reflects the (unphysical) absence of the heat flux.

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[1] The author bets a beer on *no*.

Problem 11. The physical key arguments for the non-existence result are the sign of the entropy jump and the enthalpy jump, respectively. We have shown this for water and assume these properties to hold for many substances. Are there substances where these relations do not hold?

Problem 12. The proof of the main result in Chapter 6 relies on a suited approximation of the saturation line of water given by the *IAPWS-IF97*. Is there another proof directly comparing the slope of the shock curve with the slope of the saturation curve given by the Clausius-Clapeyron equation.

Appendix

8 Appendix: Concepts

8.1 Calculus of Moving Surfaces

The aim of the present section is to *briefly* summarize the most important results for moving surfaces used throughout this work. We exemplary refer to the works by Aris [2], Dziuk et al. [26], Grinfeld [34] and the references therein.
In the following we will use the following notational conventions

(i) Lower case Greek indices refer to the surface and may take the values $\{1, 2\}$. In contrast lower case Latin indices refer to the ambient space, i.e. the standard $\mathbb{R}^3$ in our case.

(ii) Bold quantities refer to vectors in $\mathbb{R}^3$.

(iii) We use the Einstein summation convention, i.e. summation applies to every index which appears twice. Once as superscript and once as subscript. Such an index is often called *dummy index* and may be renamed. See the following two examples

$$\mathbf{x} \cdot \mathbf{y} = \sum_{i=1}^{3} x_i y_i = x^i y_i = x^j y_j,$$
$$A^\alpha B_\alpha = A^\beta B_\beta = A^1 B_1 + A^2 B_2.$$

(iv) An expression of the form $A^\alpha B_\alpha$ consisting of a *contravariant* and a *covariant tensor*[1] is called *contraction* [2].

A two dimensional surface $\mathcal{S}$ in $\mathbb{R}^3$ may be described through a parametrization depending on a two dimensional coordinate system. We want to specify this in the following. Let $\mathcal{U} \subset \mathbb{R}^2$ be open and $\Phi : \mathcal{U} \to \mathbb{R}^3$ an (injective) smooth parametrization such that

$$\mathcal{S} \equiv \Phi(\mathcal{U}) = \left\{ \mathbf{x} \in \mathbb{R}^3 \,|\, \mathbf{x} = \Phi(u^1, u^2),\; u^\alpha \in \mathcal{U},\; \alpha = 1,2 \right\}. \tag{8.1}$$

The tangents and the normal of $\mathcal{S}$ are given by

$$\boldsymbol{\tau}_\alpha = \frac{\partial \Phi}{\partial u^\alpha},\; \alpha = 1,2 \quad \text{and} \quad \boldsymbol{\nu} = \frac{\boldsymbol{\tau}_1 \times \boldsymbol{\tau}_2}{|\boldsymbol{\tau}_1 \times \boldsymbol{\tau}_2|}. \tag{8.2}$$

Since we want the tangents to be linearly independent the Jacobian of Φ should be of rank two. The components of the surface metric are given by

$$g_{\alpha\beta} = \boldsymbol{\tau}_\alpha \cdot \boldsymbol{\tau}_\beta. \tag{8.3}$$

Thus the metric is positive definite and symmetric. The inverse of the metric is denoted by $g^{\alpha\beta}$ and we further have

$$g^{\alpha\beta} g_{\beta\gamma} = \delta^\alpha_\gamma \quad \text{and} \quad g := \det(g_{\alpha\beta}) = g_{11} g_{22} - g_{12}^2. \tag{8.4}$$

A straight forward (and tedious) calculation shows

$$\sqrt{g} = |\boldsymbol{\tau}_1 \times \boldsymbol{\tau}_2|. \tag{8.5}$$

Another important observation is that a vector may be decomposed in its tangential and normal components. This is due to the fact that the surface tangents and the surface normal form a basis of $\mathbb{R}^3$. For a vector in $\mathbf{T} \in \mathbb{R}^3$ we thus may write

$$\mathbf{T} = \underbrace{T^\alpha_\tau}_{\text{tangential component}} \boldsymbol{\tau}_\alpha + \underbrace{T_\nu}_{\text{normal component}} \boldsymbol{\nu}. \tag{8.6}$$

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[1] We will skip the detailed introduction of tensors here and refer to the afore mentioned literature. A tensor is a quantity which has certain transformation properties. The order of a tensor is given by the number of indices. A tensor with upper indices is called *contravariant* and *covariant* with lower indices, respectively.

[2] Whereas tensors might change with the coordinate system a contraction produces an invariant quantity and thus it is one of the fundamental operations in tensor calculus.

When we move along the surface the tangents and the normal will change with respect to the coordinate lines. First we want to discuss the tangents. From geometric intuition it is clear that in general the tangent will change tangential and normal direction. Thus we define according to (8.6)

$$\frac{\partial \boldsymbol{\tau}_\alpha}{\partial u^\beta} = \Gamma^\gamma_{\alpha\beta} \boldsymbol{\tau}_\gamma + b_{\alpha\beta} \boldsymbol{\nu}. \tag{8.7}$$

The normal component is called *curvature tensor* and is given by

$$b_{\alpha\beta} = \frac{\partial \boldsymbol{\tau}_\alpha}{\partial u^\beta} \cdot \boldsymbol{\nu} = \frac{\partial^2 \Phi}{\partial u^\alpha \partial u^\beta} \boldsymbol{\nu}. \tag{8.8}$$

Roughly speaking it gives the change of the tangent vectors in normal direction along the coordinate lines. Again the geometric view is quite clear since we expect no normal component of the derivative of a tangent for a flat surface. Along with the curvature tensor one can define the quantity K_M which denotes the *mean curvature* [3]. It is given by

$$K_M = \frac{1}{2} g^{\alpha\beta} b_{\alpha\beta}. \tag{8.9}$$

The tangential component in (8.7) is called the *Christoffel symbol*. It can be calculated using the following formula

$$\begin{aligned}
\frac{\partial \boldsymbol{\tau}_\alpha}{\partial u^\beta} = \Gamma^\gamma_{\alpha\beta} \boldsymbol{\tau}_\gamma + b_{\alpha\beta} \boldsymbol{\nu} \quad &\overset{|\cdot \boldsymbol{\tau}_\delta \,\&|\, g^{\delta\varepsilon}}{\Leftrightarrow} \quad g^{\delta\varepsilon} \frac{\partial \boldsymbol{\tau}_\alpha}{\partial u^\beta} \cdot \boldsymbol{\tau}_\delta = \Gamma^\gamma_{\alpha\beta} g_{\gamma\delta} g^{\delta\varepsilon} = \Gamma^\varepsilon_{\alpha\beta} \\
g^{\delta\varepsilon} \frac{\partial \boldsymbol{\tau}_\alpha}{\partial u^\beta} \cdot \boldsymbol{\tau}_\delta &= \frac{1}{2} g^{\delta\varepsilon} \left(\frac{\partial \boldsymbol{\tau}_\alpha}{\partial u^\beta} \cdot \boldsymbol{\tau}_\delta + \frac{\partial \boldsymbol{\tau}_\alpha}{\partial u^\beta} \cdot \boldsymbol{\tau}_\delta \right) = \frac{1}{2} g^{\delta\varepsilon} \left(\frac{\partial \boldsymbol{\tau}_\alpha}{\partial u^\beta} \cdot \boldsymbol{\tau}_\delta + \frac{\partial \boldsymbol{\tau}_\beta}{\partial u^\alpha} \cdot \boldsymbol{\tau}_\delta \right) \\
&= \frac{1}{2} g^{\delta\varepsilon} \left(\frac{\partial (\boldsymbol{\tau}_\alpha \cdot \boldsymbol{\tau}_\delta)}{\partial u^\beta} - \frac{\partial \boldsymbol{\tau}_\delta}{\partial u^\beta} \cdot \boldsymbol{\tau}_\alpha + \frac{\partial (\boldsymbol{\tau}_\beta \cdot \boldsymbol{\tau}_\delta)}{\partial u^\alpha} - \frac{\partial \boldsymbol{\tau}_\delta}{\partial u^\alpha} \cdot \boldsymbol{\tau}_\beta \right) \\
&= \frac{1}{2} g^{\delta\varepsilon} \left(\frac{\partial g_{\alpha\delta}}{\partial u^\beta} + \frac{\partial g_{\beta\delta}}{\partial u^\alpha} - \frac{\partial (\boldsymbol{\tau}_\alpha \cdot \boldsymbol{\tau}_\beta)}{\partial u^\delta} \right) \\
\Leftrightarrow \quad \Gamma^\gamma_{\alpha\beta} &= \frac{1}{2} g^{\gamma\delta} \left(\frac{\partial g_{\alpha\delta}}{\partial u^\beta} + \frac{\partial g_{\beta\delta}}{\partial u^\alpha} - \frac{\partial g_{\alpha\beta}}{\partial u^\delta} \right). \qquad (8.10)
\end{aligned}$$

It is a non-trivial fact and observation that the curvature tensor and the Christoffel symbol are quantities which are intrinsic to the surface, see [2, 34].

---

[3] The factor 1/2 is a convention one has to agree on. It is also possible to define the mean curvature without this factor, cf. [34].

Now we discuss how the change of the (unit) normal can be calculated. Intuitively there should be no normal component and indeed this can be seen differentiating $\boldsymbol{\nu} \cdot \boldsymbol{\nu} = 1$. We therefore may write

$$\frac{\partial \boldsymbol{\nu}}{\partial u^\alpha} = T_\alpha^\beta \boldsymbol{\tau}_\beta. \tag{8.11}$$

In the following we want to determine the tangential component T_α^β, see [64]. Therefore we differentiate $\boldsymbol{\nu} \cdot \boldsymbol{\tau}_\gamma = 0$ with respect to u^α, i.e.

$$0 = \frac{\partial \boldsymbol{\nu}}{\partial u^\alpha} \cdot \boldsymbol{\tau}_\gamma + \frac{\partial \boldsymbol{\tau}_\gamma}{\partial u^\alpha} \cdot \boldsymbol{\nu} \quad \Leftrightarrow \quad \frac{\partial \boldsymbol{\nu}}{\partial u^\alpha} \cdot \boldsymbol{\tau}_\gamma = -\frac{\partial \boldsymbol{\tau}_\gamma}{\partial u^\alpha} \cdot \boldsymbol{\nu}.$$

If now (8.11) is multiplied by $\boldsymbol{\tau}_\gamma$ and compared to the previous formula we obtain

$$\frac{\partial \boldsymbol{\nu}}{\partial u^\alpha} \cdot \boldsymbol{\tau}_\gamma = T_\alpha^\beta \underbrace{\boldsymbol{\tau}_\beta \cdot \boldsymbol{\tau}_\gamma}_{=g_{\beta\gamma}} = -\frac{\partial \boldsymbol{\tau}_\gamma}{\partial u^\alpha} \cdot \boldsymbol{\nu} \quad \Leftrightarrow \quad T_\alpha^\beta = -g^{\beta\gamma} \frac{\partial \boldsymbol{\tau}_\gamma}{\partial u^\alpha} \cdot \boldsymbol{\nu}$$

Inserting this in (8.11) and using (8.7) finally gives

$$\frac{\partial \boldsymbol{\nu}}{\partial u^\alpha} = -g^{\beta\gamma} b_{\gamma\alpha} \boldsymbol{\tau}_\beta. \tag{8.12}$$

So far we only used partial derivatives with respect to the surface coordinates. This however might lead to problems since the result may depend on the chosen coordinates for some quantities. Therefore one needs a new derivative which is independent from the chosen parametrization. This is called *covariant derivative* ∇_α. We will omit the details of the derivation and interpretation and again refer to the books [2, 34]. In short one can think of the covariant derivative as respecting the change in the coordinates as well as the change with respect to the tangents. In full generality the covariant derivative for a quantity with mixed indices referring to the Euclidean $\mathbb{R}^3$ [4] and the surface we have (see [34])

$$\nabla_\gamma T^{i\alpha}_{j\beta} = \frac{\partial T^{i\alpha}_{j\beta}}{\partial u^\gamma} + \tau^k_\gamma \Gamma^i_{mk} T^{m\alpha}_{j\beta} - \tau^k_\gamma \Gamma^m_{ik} T^{i\alpha}_{m\beta} + \Gamma^\alpha_{\delta\gamma} T^{i\delta}_{j\beta} - \Gamma^\delta_{\gamma\beta} T^{i\alpha}_{j\delta}. \tag{8.13}$$

---

[4] Here we assumed the canonical basis, otherwise a slight generalization is necessary, see [34].

The basic rules are that for every upper index one has an + Christoffel term and a − for every lower index. If an index does not appear the whole Christoffel term vanishes, e.g.

$$\nabla_\gamma T^\alpha = \frac{\partial T^\alpha}{\partial u^\gamma} + \Gamma^\alpha_{\delta\gamma} T^\delta.$$

The covariant derivative has the following properties (more may be found in the given literature)

(i) The covariant derivative coincides with the partial derivative when applied to invariants (e.g. the normal $\boldsymbol{\nu}$ and its components).

(ii) The covariant derivative satisfies sum and product rules, but it does not commute.

(iii) The covariant derivative commutes with contraction.

(iv) The covariant derivatives $\nabla_\gamma g_{\alpha\beta}$ and $\nabla_\gamma g^{\alpha\beta}$ vanish. This is also called *metrilinic property*, see [34].

As mentioned above the surface normal is an invariant and thus [5]

$$\nabla_\alpha \boldsymbol{\nu} = \frac{\partial \boldsymbol{\nu}}{\partial u^\alpha}.$$

For the tangents we obtain

$$\nabla_\beta \boldsymbol{\tau}_\alpha = \frac{\partial \boldsymbol{\tau}_\alpha}{\partial u^\beta} + \Gamma^\gamma_{\alpha\beta} \boldsymbol{\tau}_\gamma \overset{(8.7)}{=} b_{\alpha\beta} \boldsymbol{\nu}. \tag{8.14}$$

In this result the main property of the covariant derivative becomes apparent, i.e. the result is independent from the chosen parametrization of the surface. Further we have that $\nabla_\beta \boldsymbol{\tau}_\alpha = \nabla_\alpha \boldsymbol{\tau}_\beta$.

Using the covariant derivative one can also calculate the surface divergence of a quantity T^α as (see [34])

$$\nabla_\alpha T^\alpha = \frac{1}{\sqrt{g}} \frac{\partial}{\partial u^\alpha} \left(\sqrt{g} T^\alpha \right). \tag{8.15}$$

---

[5] This can be seen by comparing the result obtained above (8.12) to the derivation of $\nabla_\alpha \boldsymbol{\nu}$ in [34].

Another important relation my be obtained by calculating the covariant derivative of (8.6)

$$\begin{aligned}
\nabla_\alpha \mathbf{T} &= \nabla_\alpha \left(T_\tau^\beta \boldsymbol{\tau}_\beta + T_\nu \boldsymbol{\nu} \right) = \nabla_\alpha \left(T_\tau^\beta \boldsymbol{\tau}_\beta \right) + \nabla_\alpha \left(T_\nu \boldsymbol{\nu} \right) \\
&= \boldsymbol{\tau}_\beta \nabla_\alpha T_\tau^\beta + T_\tau^\beta \nabla_\alpha \boldsymbol{\tau}_\beta + \boldsymbol{\nu} \nabla_\alpha T_\nu + T_\nu \nabla_\alpha \boldsymbol{\nu} \\
&= \boldsymbol{\tau}_\beta \nabla_\alpha T_\tau^\beta + T_\tau^\beta b_{\alpha\beta} \boldsymbol{\nu} + \frac{\partial T_\nu}{\partial u^\alpha} \boldsymbol{\nu} - T_\nu g^{\beta\gamma} b_{\gamma\alpha} \boldsymbol{\tau}_\beta \\
&= \left(\nabla_\alpha T_\tau^\beta - T_\nu g^{\beta\gamma} b_{\gamma\alpha} \right) \boldsymbol{\tau}_\beta + \left(T_\tau^\beta b_{\alpha\beta} + \frac{\partial T_\nu}{\partial u^\alpha} \right) \boldsymbol{\nu}. \qquad (8.16)
\end{aligned}$$

Equations (8.6) and (8.16) are also valid for tensorial quantities $\mathbf{T}^\alpha$, i.e.

$$\mathbf{T}^\alpha = T_\tau^{\alpha\beta} \boldsymbol{\tau}_\beta + T_\nu^\alpha \boldsymbol{\nu} \quad \text{and} \quad \nabla_\gamma \mathbf{T}^\alpha = \left(\nabla_\gamma T_\tau^{\alpha\beta} - T_\nu^\alpha g^{\beta\delta} b_{\delta\gamma} \right) \boldsymbol{\tau}_\beta + \left(T_\tau^{\alpha\beta} b_{\gamma\beta} + \nabla_\gamma T_\nu^\alpha \right) \boldsymbol{\nu}. \qquad (8.17)$$

So far we only considered a fixed surface $\mathcal{S} \subset \mathbb{R}^3$. Now we wan to extend the results to a moving surface. A moving surface $\mathcal{S}(t)$ can be considered as a family of surfaces $S(t)$ with a parameter $t \in [0, T_0], T_0 > 0$. The initial surface $\mathcal{S}_0 = \mathcal{S}(0)$ may be described as before with a smooth injective parametrization $\Phi : \mathcal{U} \to \mathcal{S}_0$. We further assume that there exists a suited velocity field $\mathbf{w}(t, .)$ and a consistent diffeomorphism $\Psi(t, .)$ such that the following holds

$$\Psi(t, .) : \mathcal{S}_0 \to \mathcal{S}(t) \quad \text{with} \quad \begin{cases} \dfrac{\partial}{\partial t} \Psi(t, .) = \mathbf{w}(t, \Psi(t, .)) \\ \Psi(0, .) = \mathrm{Id} \end{cases} .$$

With this we have for every particle P with $\mathbf{x}_P(0) = \mathbf{x}_0 \in \mathcal{S}_0$ that $\mathbf{x}_P(t) = \Psi(t, \mathbf{x}_P(0)) \in \mathcal{S}(t)$ and equivalently

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t} \mathbf{x}_p(t) = \mathbf{w}(t, \mathbf{x}_P(t)) \\ \mathbf{x}_P(0) = \mathbf{x}_0. \end{cases}$$

Now we may also describe the surface $\mathcal{S}(t)$ in terms of the surface coordinates $(u^1, u^2) \in \mathcal{U}$ using the mapping

$$\tilde{\Phi} = \Psi(t, .) \circ \Phi : \mathcal{U} \to \mathcal{S}(t).$$

The results obtained so far remain valid and we assume that the dependence on the parameter t is smooth. The first immediate result we obtain is that the *coordinate velocity* of a point $\mathbf{x}$ is given by [6]

$$\mathbf{w} = \frac{\partial \tilde{\Phi}(t, u^\alpha)}{\partial t}. \tag{8.18}$$

and my be decomposed according to (8.6)

$$\mathbf{w} = w_\tau^\alpha \boldsymbol{\tau}_\alpha + w_\nu \boldsymbol{\nu}. \tag{8.19}$$

The quantities w_τ^α are called *tangential coordinate velocity*. The term w_ν is called *velocity of the surface* with $w_\nu \boldsymbol{\nu}$ being the *vector normal velocity*, see [34]. It is important to note that w_ν is an invariant of the surface and a nice geometric motivation is given in [34]. Now we can relate the coordinate velocity (8.18) and the tangents $(8.2)_1$ by

$$\frac{\partial \boldsymbol{\tau}_\alpha}{\partial t} = \frac{\partial \mathbf{w}}{\partial u^\alpha}. \tag{8.20}$$

The covariant derivative of the velocity can be obtained using (8.16)

$$\nabla_\alpha \mathbf{w} = \left(\nabla_\alpha w_\tau^\beta - w_\nu g^{\beta\gamma} b_{\gamma\alpha}\right) \boldsymbol{\tau}_\beta + \left(w_\tau^\beta b_{\alpha\beta} + \frac{\partial w_\nu}{\partial u^\alpha}\right) \boldsymbol{\nu}. \tag{8.21}$$

A small computation (involving some index changes) shows that

$$\nabla_\alpha \mathbf{w} = \frac{\partial \mathbf{w}}{\partial u^\alpha}.$$

With this we may calculate the time derivative of the metric $g_{\alpha\beta}$

$$\begin{aligned}
\frac{\partial}{\partial t} g_{\alpha\beta} &= \frac{\partial}{\partial t}(\boldsymbol{\tau}_\alpha \cdot \boldsymbol{\tau}_\beta) = \frac{\partial \boldsymbol{\tau}_\alpha}{\partial t} \cdot \boldsymbol{\tau}_\beta + \boldsymbol{\tau}_\alpha \cdot \frac{\partial \boldsymbol{\tau}_\beta}{\partial t} = \nabla_\alpha \mathbf{w} \cdot \boldsymbol{\tau}_\beta + \boldsymbol{\tau}_\alpha \cdot \nabla_\beta \mathbf{w} \\
&= \left(\nabla_\alpha w_\tau^\gamma - w_\nu g^{\gamma\delta} b_{\delta\alpha}\right) \boldsymbol{\tau}_\gamma \cdot \boldsymbol{\tau}_\beta + \left(\nabla_\beta w_\tau^\gamma - w_\nu g^{\gamma\delta} b_{\gamma\beta}\right) \boldsymbol{\tau}_\gamma \cdot \boldsymbol{\tau}_\alpha \\
&= g_{\gamma\beta} \nabla_\alpha w_\tau^\gamma + g_{\gamma\alpha} \nabla_\beta w_\tau^\gamma - 2 w_\nu b_{\alpha\beta}.
\end{aligned} \tag{8.22}$$

---

[6] A major issue when working with moving surfaces is how to define an invariant time derivative. Here we only refer to the result obtained in [13, 26, 34, 35] since we are not concerned with the details.

If we contract (8.22) with the inverse $g^{\alpha\beta}$ one yields

$$\begin{aligned} g^{\alpha\beta}\frac{\partial}{\partial t}g_{\alpha\beta} &= g^{\alpha\beta}\left(g_{\gamma\beta}\nabla_\alpha w_\tau^\gamma + g_{\gamma\alpha}\nabla_\beta w_\tau^\gamma - 2w_\nu b_{\alpha\beta}\right) \\ &= \delta_\gamma^\alpha \nabla_\alpha w_\tau^\gamma + \delta_\gamma^\beta \nabla_\beta w_\tau^\gamma - 2w_\nu g^{\alpha\beta} b_{\alpha\beta} \\ &= 2\left(\nabla_\alpha w_\tau^\alpha - 2w_\nu K_M\right). \end{aligned} \tag{8.23}$$

Now we can also calculate the time derivative of the determinant g. There are two possible ways to obtain the result. First one may use the non-trivial result (see [34]) that

$$\frac{\partial g}{\partial g_{\alpha\beta}} = g g^{\alpha\beta}.$$

Now one obtains using the chain rule and (8.23)

$$\frac{\partial}{\partial t}g = \frac{\partial g}{\partial g_{\alpha\beta}}\frac{\partial}{\partial t}g_{\alpha\beta} = g g^{\alpha\beta}\frac{\partial}{\partial t}g_{\alpha\beta} = 2g\left(\nabla_\alpha w_\tau^\alpha - 2w_\nu K_M\right). \tag{8.24}$$

Second we follow the more direct approach presented in [2], i.e.

$$\begin{aligned} \frac{\partial}{\partial t}g = \frac{\partial}{\partial t}\left(g_{11}g_{22} - g_{12}^2\right) &= g_{22}\frac{\partial}{\partial t}g_{11} + g_{11}\frac{\partial}{\partial t}g_{22} - 2g_{12}\frac{\partial}{\partial t}g_{12} \\ &= g g^{11}\frac{\partial}{\partial t}g_{11} + g g^{22}\frac{\partial}{\partial t}g_{22} + 2g g^{12}\frac{\partial}{\partial t}g_{12} = g g^{\alpha\beta}\frac{\partial}{\partial t}g_{\alpha\beta}. \end{aligned}$$

A further useful relation connects $\nabla_\alpha \mathbf{w}$ and the time derivative of the metric in a special situation. Therefore we consider $A^{\alpha\beta}\boldsymbol{\tau}_\beta$ with a symmetric tensor $A^{\alpha\beta} = A^{\beta\alpha}$. Now we calculate

$$\begin{aligned} A^{\alpha\beta}\boldsymbol{\tau}_\beta \cdot \nabla_\alpha \mathbf{w} &\overset{(8.20)}{=} A^{\alpha\beta}\boldsymbol{\tau}_\beta \cdot \frac{\partial \boldsymbol{\tau}_\alpha}{\partial t} = \frac{1}{2}\left(A^{\alpha\beta}\boldsymbol{\tau}_\beta \cdot \frac{\partial \boldsymbol{\tau}_\alpha}{\partial t} + A^{\alpha\beta}\boldsymbol{\tau}_\beta \cdot \frac{\partial \boldsymbol{\tau}_\alpha}{\partial t}\right) \\ &= \frac{1}{2}\left(A^{\alpha\beta}\boldsymbol{\tau}_\beta \cdot \frac{\partial \boldsymbol{\tau}_\alpha}{\partial t} + A^{\beta\alpha}\boldsymbol{\tau}_\alpha \cdot \frac{\partial \boldsymbol{\tau}_\beta}{\partial t}\right) \\ &\overset{A^{\alpha\beta}=A^{\beta\alpha}}{=} \frac{1}{2}A^{\alpha\beta}\left(\boldsymbol{\tau}_\beta \cdot \frac{\partial \boldsymbol{\tau}_\alpha}{\partial t} + \boldsymbol{\tau}_\alpha \cdot \frac{\partial \boldsymbol{\tau}_\beta}{\partial t}\right) \\ &= \frac{1}{2}A^{\alpha\beta}\frac{\partial}{\partial t}g_{\alpha\beta}. \end{aligned} \tag{8.25}$$

9 Appendix: Isothermal Case

9.1 Detailed Calculations for the Isothermal Case - Analysis

In this short appendix we want to give the detailed calculation used in the proof of Lemma 3.3.1. There we started with

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}p_V}\left(p_V^* h(p_V^*, p_L^*)\,[\![v]\!]\right) &= \partial_{p_V}\left(p_V^* h(p_V^*, p_L^*)\,[\![v]\!]\right) + \partial_{p_L}\left(p_V^* h(p_V^*, p_L^*)\,[\![v]\!]\right)\varphi'(p_V^*)\\ &= \left(h(p_V^*, p_L^*) + p_V^*\partial_{p_V} h(p_V^*, p_L^*)\right)[\![v]\!] + p_V^* h(p_V^*, p_L^*)\frac{v_V^2}{a_V^2}\\ &\quad+ \left\{p_V^*\partial_{p_L} h(p_V^*, p_L^*)\,[\![v]\!] - p_V^* h(p_V^*, p_L^*)\frac{v_L^2}{a_L^2}\right\}\varphi'(p_V^*).\end{aligned}$$

We assume $p_V^* h(p_V^*, p_L^*) \neq 0$ from now on and thus may write

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}p_V}\left(p_V^* h(p_V^*, p_L^*)\,[\![v]\!]\right) &= \frac{1}{2p_V^* h(p_V^*, p_L^*)}\left(\partial_{p_V} f(p_V^*, p_L^*) + 1\right) + \frac{1}{2}p_V^* h(p_V^*, p_L^*)\frac{v_V^2}{a_V^2}\\ &+ \left\{\frac{1}{2p_V^* h(p_V^*, p_L^*)}\left(\partial_{p_L} f(p_V^*, p_L^*) - 1\right) - \frac{1}{2}p_V^* h(p_V^*, p_L^*)\frac{v_L^2}{a_L^2}\right\}\varphi'(p_V^*).\end{aligned}$$

Multiplication with $\partial_{p_L} f(p_V^*, p_L^*) > 0$ and use of

$$\varphi'(p_V^*) = -\frac{\partial_{p_V} f(p_V^*, p_L^*)}{\partial_{p_L} f(p_V^*, p_L^*)}.$$

gives

$$
\begin{aligned}
&\partial_{p_L} f(p_V^*, p_L^*) \frac{\mathrm{d}}{\mathrm{d}p_V}\left(p_V^* h(p_V^*, p_L^*) \llbracket v \rrbracket\right) = \dots \\
&= \left\{ \frac{1}{2p_V^* h(p_V^*, p_L^*)} (\partial_{p_V} f(p_V^*, p_L^*) + 1) + \frac{1}{2} p_V^* h(p_V^*, p_L^*) \frac{v_V^2}{a_V^2} \right\} \partial_{p_L} f(p_V^*, p_L^*) \\
&- \left\{ \frac{1}{2p_V^* h(p_V^*, p_L^*)} (\partial_{p_L} f(p_V^*, p_L^*) - 1) - \frac{1}{2} p_V^* h(p_V^*, p_L^*) \frac{v_L^2}{a_L^2} \right\} \partial_{p_V} f(p_V^*, p_L^*) \\
&= \frac{1}{2p_V^* h(p_V^*, p_L^*)} (\partial_{p_V} f(p_V^*, p_L^*) + \partial_{p_L} f(p_V^*, p_L^*)) \\
&+ \frac{1}{2} p_V^* h(p_V^*, p_L^*) \left(\partial_{p_V} f(p_V^*, p_L^*) \frac{v_L^2}{a_L^2} + \partial_{p_L} f(p_V^*, p_L^*) \frac{v_V^2}{a_V^2} \right) \\
&= (h(p_V^*, p_L^*) + p_V \partial_{p_V} h(p_V^*, p_L^*)) \left(1 + (p_V^* h(p_V^*, p_L^*))^2 \frac{v_L^2}{a_L^2} \right) \llbracket v \rrbracket \\
&+ p_V \partial_{p_L} h(p_V^*, p_L^*) \left(1 + (p_V^* h(p_V^*, p_L^*))^2 \frac{v_V^2}{a_V^2} \right) \llbracket v \rrbracket + p_V^* h(p_V^*, p_L^*) \left(\frac{v_V^2}{a_V^2} - \frac{v_L^2}{a_L^2} \right) \\
&= h(p_V^*, p_L^*) \llbracket v \rrbracket \left(1 + (p_V^* h(p_V^*, p_L^*))^2 \frac{v_L^2}{a_L^2} \right) - p_V^* h(p_V^*, p_L^*) \left\llbracket \frac{v^2}{a^2} \right\rrbracket \\
&+ \tau p_V \llbracket v \rrbracket^2 \left(1 - (p_V^* h(p_V^*, p_L^*))^4 \frac{v_V^2}{a_V^2} \frac{v_L^2}{a_L^2} \right) \\
&= h(p_V^*, p_L^*) \left(\llbracket v \rrbracket + \llbracket v \rrbracket (p_V^* h(p_V^*, p_L^*))^2 \frac{v_L^2}{a_L^2} - p_V^* \left\llbracket \frac{v^2}{a^2} \right\rrbracket \right) \\
&+ \tau p_V \llbracket v \rrbracket^2 \left(1 - (p_V^* h(p_V^*, p_L^*))^4 \frac{v_V^2}{a_V^2} \frac{v_L^2}{a_L^2} \right)
\end{aligned}
$$

Thus we finally obtain the following equation

$$
\begin{aligned}
\partial_{p_L} f(p_V^*, p_L^*) \frac{\mathrm{d}}{\mathrm{d}p_V}\left(p_V^* h(p_V^*, p_L^*) \llbracket v \rrbracket\right) &= h(p_V^*, p_L^*) \left(v_L \left(1 - \frac{p_L^* v_L}{a_L^2} \right) - v_V \left(1 - \frac{p_V^* v_V}{a_V^2} \right) \right) \\
&\quad + \tau p_V \llbracket v \rrbracket^2 \left(1 - (p_V^* h(p_V^*, p_L^*))^4 \frac{v_V^2}{a_V^2} \frac{v_L^2}{a_L^2} \right).
\end{aligned}
$$

9.2 Detailed Calculations for the Isothermal Case - Numerics

In this section we want to give the derivatives and some calculations needed throughout Chapter 4. All quantities and assumptions are as in the Chapters 3 and 4.

9.2.1 Derivatives of $h(p_V, p_L)$ and $f(p_V, p_L)$ with respect to p_L

The derivatives of (3.40)$_1$

$$\begin{aligned} h(p_V, p_L) &:= \tau \left[\!\left[g - \frac{1}{2} p(v_L + v_V) \right]\!\right] \\ &= \tau \left[g_L(p_L) - g_V(p_V) - \frac{1}{2}(p_L - p_V)(v_L(p_L) + v_V(p_V)) \right] \end{aligned}$$

with respect to p_L are

$$\partial_{p_L} h(p_V, p_L) = \frac{\tau}{2} \left[[\![v]\!] + [\![p]\!] \frac{v_L^2}{a_L^2} \right], \tag{9.1}$$

$$\partial_{p_L}^2 h(p_V, p_L) = -\tau [\![p]\!] \frac{v_L^3}{a_L^4} \mathcal{G}_L, \tag{9.2}$$

$$\partial_{p_L}^3 h(p_V, p_L) = -\tau \frac{v_L^3}{a_L^4} \mathcal{G}_L - \tau [\![p]\!] \frac{v_L^4}{a_L^6} \mathcal{G}_L (1 - 4\mathcal{G}_L) - \tau [\![p]\!] \frac{v_L^3}{a_L^4} \frac{\partial \mathcal{G}_L}{\partial p_L}. \tag{9.3}$$

Note that for the third derivative (9.3) the derivative of $\mathcal{G}_L$ is needed. Up to our knowledge this term has not been discussed in the literature so far. Which is presumably due to the fact that this is a rather technical quantity which is not needed in most cases. However, in many cases it might be sufficient to work with $\mathcal{G}_L = const.$ which then simplifies the calculations.

The derivatives of (3.40)$_2$

$$f(p_V, p_L) := [\![p]\!] + (p_V h(p_V, p_L))^2 [\![v]\!]$$

with respect to p_L are given in the following. For the derivatives of first and second order we yield

$$\partial_{p_L} f(p_V, p_L) = 1 + 2(p_V h(p_V, p_L))(p_V \partial_{p_L} h(p_V, p_L)) [\![v]\!] - (p_V h(p_V, p_L))^2 \left(\frac{v_L}{a_L}\right)^2, \tag{9.4}$$

$$\begin{aligned}\partial^2_{p_L} f(p_V, p_L) = {} & 2(p_V h(p_V, p_L)) \left(p_V \partial^2_{p_L} h(p_V, p_L)\right) [\![v]\!] + 2 \left(p_V \partial_{p_L} h(p_V, p_L)\right)^2 [\![v]\!] \\ & - 4(p_V h(p_V, p_L)) \left(p_V \partial_{p_L} h(p_V, p_L)\right) \left(\frac{v_L}{a_L}\right)^2 + 2(p_V h(p_V, p_L)^2 \frac{v_L^3}{a_L^4} \mathcal{G}_L,\end{aligned} \tag{9.5}$$

The third order derivative is needed for the remainder of the expansion and is given by

$$\begin{aligned} & \partial^3_{p_L} f(p_V, p_L) = \dots \\ & = 2(p_V h(p_V, p_L)) \left(p_V \partial^3_{p_L} h(p_V, p_L\right) [\![v]\!] + 6 \left(p_V \partial_{p_L} h(p_V, p_L)\right) \left(p_V \partial^2_{p_L} h(p_V, p_L)\right) [\![v]\!] \\ & - 6(p_V h(p_V, p_L)) \left(p_V \partial^2_{p_L} h(p_V, p_L)\right) \left(\frac{v_L}{a_L}\right)^2 - 2 \left(p_V \partial^2_{p_L} h(p_V, p_L)\right)^2 \left(\frac{v_L}{a_L}\right)^2 \\ & - 4 \left(p_V \partial_{p_L} h(p_V, p_L)\right)^2 \left(\frac{v_L}{a_L}\right)^2 + 12(p_V h(p_V, p_L)) \left(p_V \partial_{p_L} h(p_V, p_L)\right) \frac{v_L^3}{a_L^4} \mathcal{G}_L \\ & + 2(p_V h(p_V, p_L))^2 \frac{v_L^4}{a_L^6} \mathcal{G}_L \, (1 - 4\mathcal{G}_L) + 2(p_V h(p_V, p_L))^2 \frac{v_L^3}{a_L^4} \frac{\partial \mathcal{G}_L}{\partial p_L}. \end{aligned} \tag{9.6}$$

Concerning the third derivative (9.6) the same remark as before applies to the derivative of $\mathcal{G}_L$.

9.2.2 Limit behaviour as $p_V \to 0$

Here we want to present the details for the result (4.19) in the case that the vapor phase is modeled as an ideal Gas. For $h(p_V, p_0)$ and $\partial_{p_L} h(p_V, p_0)$ we have the following limits

$$
\begin{aligned}
\lim_{p_V \to 0} p_V h(p_V, p_0) &= \lim_{p_V \to 0} \tau p_V \left[-g_V(p_V) - \frac{1}{2}(p_0 - p_V)(v_L(p_0) + v_V(p_V)) \right] \\
&= -\tau \lim_{p_V \to 0} \left[\underbrace{a_V^2 p_V \ln \frac{p_V}{p_0}}_{\to 0} + \underbrace{\frac{p_V}{2}(p_0 - p_V)\,(v_{L0} + v_V)}_{\to p_0 a_v^2/2} \right] \\
&= -\frac{1}{2}\tau p_0 a_V^2, && (9.7) \\
\lim_{p_V \to 0} p_V \partial_{p_L} h(p_V, p_0) &= \lim_{p_V \to 0} \frac{\tau p_V}{2} \left[(v_L(p_0) - v_V(p_V)) + (p_0 - p_V) \left(\frac{v_L(p_0)}{a_L(p_0)} \right)^2 \right] \\
&= \frac{\tau}{2} \lim_{p_V \to 0} \left[\underbrace{p_V\,(v_{L0} - v_V)}_{\to -a_V^2} + \underbrace{p_V (p_0 - p_V) \left(\frac{v_{L0}}{a_{L0}} \right)^2}_{\to 0} \right] \\
&= -\frac{1}{2}\tau a_V^2, && (9.8) \\
\lim_{p_V \to 0} \partial_{p_L}^2 h(p_V, p_0) &= -\tau \lim_{p_V \to 0} (p_0 - p_V) \frac{v_{L0}^3}{a_{L0}^4} \mathcal{G}_{L0} = -\tau p_0 \frac{v_{L0}^3}{a_{L0}^4} \mathcal{G}_{L0}. && (9.9)
\end{aligned}
$$

The limits of the functions (3.40)$_2$, (9.4) and (9.5) all diverge to minus infinity for $p_V \to 0$ and $p_L = p_0$. Here we need the limits of the quotients appearing in (4.17). We first yield (omitting the arguments (p_V, p_0) of the occurring functions)

$$
\begin{aligned}
&\lim_{p_V \to 0} \frac{f(p_V, p_0)}{\partial_{p_L}^2 f(p_V, p_0)} = \dots \\
&= \lim_{p_V \to 0} \frac{p_0 - p_V + (p_V h)^2\,(v_{L0} - v_V)}{2 p_V^2 h \partial_{p_L}^2 h\, [\![v]\!] + 2 \left(p_V \partial_{p_L} h \right)^2 [\![v]\!] - 4 p_V^2 h \partial_{p_L} h \left(\frac{v_{L0}}{a_{L0}} \right)^2 + 2 (p_V h)^2 \frac{v_{L0}^3}{a_{L0}^4} \mathcal{G}_{L0}} \\
&= \lim_{p_V \to 0} \frac{(p_V h)^2}{2 (p_V \partial_{p_L} h)^2} = \frac{p_0^2}{2} && (9.10)
\end{aligned}
$$

and further

$$
\begin{aligned}
&\lim_{p_V\to 0} \frac{\partial_{p_L} f(p_V,p_0)}{\partial^2_{p_L} f(p_V,p_0)} = \dots \\
= &\lim_{p_V\to 0} \frac{1 + 2(p_V h)\left(p_V \partial_{p_L} h\right)[\![v]\!] - (p_V h)^2\left(\frac{v_{L0}}{a_{L0}}\right)^2}{2p_V^2 h \partial^2_{p_L} h\,[\![v]\!] + 2\left(p_V \partial_{p_L} h\right)^2[\![v]\!] - 4p_V^2 h \partial_{p_L} h\left(\frac{v_{L0}}{a_{L0}}\right)^2 + 2(p_V h)^2 \frac{v_{L0}^3}{a_{L0}^4}\mathcal{G}_{L0}} \\
= &\lim_{p_V\to 0} \frac{2(p_V h)\left(p_V \partial_{p_L} h\right)}{2\left(p_V \partial_{p_L} h\right)^2} = \lim_{p_V\to 0} \frac{p_V h}{p_V \partial_{p_L} h} = p_0.
\end{aligned}
\tag{9.11}
$$

Here we have also used that $[\![v]\!] \to -\infty$ for $p_V \to 0$ and $p_L = p_0$ for an ideal gas. Now we can show

$$
\begin{aligned}
&\lim_{p_V\to 0} \tilde{\varphi}(p_V) = \dots \\
= &\lim_{p_V\to 0}\left[p_0 - \frac{\partial_{p_L} f(p_V,p_0)}{\partial^2_{p_L} f(p_V,p_0)} - \sqrt{\frac{\left(\partial_{p_L} f(p_V,p_0)\right)^2 - 2f(p_V,p_0)\partial^2_{p_L} f(p_V,p_0)}{\left(\partial^2_{p_V} f(p_V,p_0)\right)^2}}\right] \\
= &\, p_0 - \lim_{p_V\to 0} \frac{\partial_{p_L} f(p_V,p_0)}{\partial^2_{p_L} f(p_V,p_0)} - \sqrt{\left(\lim_{p_V\to 0} \frac{\partial_{p_L} f(p_V,p_0)}{\partial^2_{p_L} f(p_V,p_0)}\right)^2 - 2\lim_{p_V\to 0} \frac{f(p_V,p_0)}{\partial^2_{p_L} f(p_V,p_0)}} = 0.
\end{aligned}
\tag{9.12}
$$

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