Modeling and Analysis of District Heating Networks with Applications in Optimal Control

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Supervisors

Prof. Dr. René Pinnau, TU Kaiserslautern

Dr. Jan Mohring, Fraunhofer ITWM Kaiserslautern

First examiner

Prof. Dr. René Pinnau, TU Kaiserslautern

Second examiner

Prof. Dr. Simone Göttlich, Univ. Mannheim

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Kaiserslautern, 30. Juni 2022 Dominik Linn

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Contents

Abstract

This thesis deals with modeling and simulation of district heating networks (DHN) and the mathematical analysis of the proposed DHN model. We provide a detailed derivation of the complete system of governing equations, starting from a brief exposition of the physical quantities of interest, continued with the components to set up a graph based network model accounting for fluxes and coupling conditions, the transport equations for water and thermal energy in pipelines, and the terms representing consumers and producers. On this basis, we perform an analysis of the solvability of the model equations, starting from the scalar advection problem in a single–consumer single–producer network, to a generalized problem suitable to model simple networks without loops. We also derive an abstract formulation of the problem, which serves as a rigorous mathematical model that can be utilized for optimization problems. The theoretical results can be utilized to perform transient simulations of real world DHN and optimize their performance by optimal control, as indicated in a case study.

Kurzzusammenfassung

Diese Arbeit befasst sich mit der Modellierung und Simulation von Fernwärmenetzen und der mathematischen Analyse des vorgeschlagenen Netzmodells. Nach einer kurzen Darstellung der relevanten physikalischen Größen folgt eine detaillierte Herleitung des vollständigen Gleichungssystems, welches ein Fernwärmenetz beschreibt. Wesentliche Bestandteile sind die Komponenten zur Aufstellung eines graphenbasierten Netzmodells unter Berücksichtigung von Flüssen und Kopplungsbedingungen, die Transportgleichungen für Wasser und Wärmeenergie in Rohrleitungen und die Modellterme für Verbraucher und Erzeuger. Auf dieser Grundlage führen wir eine Analyse der Lösbarkeit der Modellgleichungen durch, ausgehend vom skalaren Advektionsproblem in einem Ein-Verbraucher-Ein-Erzeuger-Netzwerk bis hin zu einem verallgemeinerten Problem, das sich für die Modellierung einfacher Netzwerke ohne Schleifen eignet. Wir leiten auch eine abstrakte Formulierung des Problems ab, die als strenges mathematisches Modell dient, das für Optimierungsprobleme verwendet werden kann. Die theoretischen Ergebnisse können genutzt werden, um instationäre Simulationen von realen Fernwärmenetzen durchzuführen und deren Leistung durch optimale Steuerung zu optimieren. Dies wird in einer Fallstudie aufgezeigt.

Publications

Optimal control of district heating networks [Linn et al., 2019]

Linn, D., Mohring, J., and Siedow N.

Proceedings in Applied Mathematics and Mechanics (2019)

doi: 10.1002/pamm.201900491

District heating networks - dynamic simulation and optimal operation [Mohring et al., 2021]

Mohring, J., Linn, D., Eimer, M., Rein, M., and Siedow, N.

Mathematical Modeling, Simulation, and Optimization for Power Engineering and Management, vol. 34, pp. 303-325 (2021)

doi: 10.1007/978-3-030-62732-4_14

Adjoint based optimal control of nonlocal advection with bilinear mixed constraints in H^1 [Linn et al., 2021]

Linn, D., Mohring, J., and Pinnau, R.

Proceedings in Applied Mathematics and Mechanics (2021)

doi: 10.1002/pamm.202100240

Chapter 1

Introduction

District heating designates the supply of heat to buildings through a heating network delivering thermal energy generated by a central supplier like e.g. a power plant, solar thermal or geothermal installation, or a large heat pump. The energy is used to heat water, which is then fed into a network of insulated pipes that transport thermal energy straight into the buildings connected to the system. The water then flows through a handover station and into the building's own heat distribution system, which provides for a supply of heating energy and hot water. Once the water has cooled down, it flows back to the original heat source and the circle begins anew (see FIGURE *1.1*). In this way, buildings that are supplied with district heating can do without their own heating systems. [1]

The climate change mitigation project *Drawdown* lists district heating technology among the most efficient methods to reduce greenhouse emissions. We refer to https://www.drawdown.org/solutions/district-heating for a discussion of the benefits and limitations of the technology.

District heating networks (DHN) will play a prominent role in sector coupling. On the one hand, they can help compensating for fluctuations in renewable power generation. On the other hand, they allow to use waste heat from industrial processes and thus save natural gas. However, this new role of district heating requires new operating modes, deeper insight into the network and, consequently, more sophisticated simulation and optimization tools.

The recent article [Mohring et al., 2021] provides a consise summary of the aspects that are relevant for the future design of DHN and their operating modes, which we reproduce in parts, as a motivation for the research work carried out in this thesis.

Modern district heating plants use combined heat and power generation. Operators can decide which part of the hot steam is used for power generation and which part for district heating. The heating network behaves more like a storage device allowing delays between feed-in and consumption. This enables the operator to react to sudden changes in the demand for electric power by redirecting temporarily the hot steam.

Another task is optimal preheating. In some periods of the year, the power of the main heating source is enough to cover the demand on average, but not during the load peaks. Here, additional gas boilers have to be fired, which is expensive due to long start-up and shut-down phases. To some extent, this can be avoided by intelligent preheating. At some point, however, the contractually guaranteed connection pressures and temperatures can no longer be maintained.

So far, operators have been able to master these tasks thanks to many years of experience. In the future, however, district heating networks will no longer be supplied by a

[1] https://www.bmwi-energiewende.de/EWD/Redaktion/EN/Newsletter/2021/03/Meldung/direkt-account.html

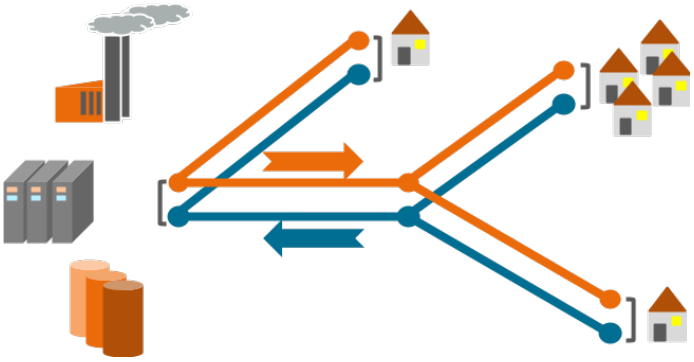

Figure 1.1: A schematic view of a district heating network, with separate forward (orange) and return flow (blue) pipe networks.

single source, but also by waste heat of industrial plants. At that point at the latest, simulation will have to be used to get an idea of the present state of the network and its future development.
Dynamic run-time effects play a central role for all of these tasks, while current software does usually not take them into account. Products for operational optimization usually treat the entire network as a sink without structure [KISTERS Gruppe, 2020]. On the other hand, thermo-hydraulic simulators are made for network design and provide only quasi-stationary solutions [Fischer-Uhrig, Ingenieurbüro, 2018]. This means that the temperature field is calculated as if the current consumption had always been the same before. In particular, no temperature fields can be represented that are warmer inside the network than at the source.
But also academic codes which are based on classical numerical methods for hyperbolic transport [Köcher, 2000] reach their limits, since the shortest pipes and highest flow velocities define the calculation grid in time and place, while smoothness of real consumption profiles is not exploited. The following example may illustrate the challenge. The city net of Technische Werke Ludwigshafen (TWL) comprises about 1000 consumers and 6000 pipes. In [Mohring et al., 2021] a periodic optimal control problem for known consumption was addressed, ignoring issues like reconstructing states from noisy measurements. In the future, however, TWL intends to apply model-predictive control. Periods of two or three days have to be simulated several times within a quarter of an hour. Using a standard first-order upwind method, due to stability, one has to deal with more than 1.9×10^9 degrees of freedom in space and time, which is far too much for solving problems in time.

1.1 Related work

Before discussing the models and methods used in this thesis, we will give a more general overview of related literature (see also [Mohring et al., 2021]). Early approaches to computer aided operational optimization of district heating networks date back to 1995 [Benonysson et al., 1995]. The authors identified the significant role of time delays in distribution networks, and the resulting complexity of an accurate numerical solution. The network dynamics are approximated using the so-called *node method* - a *Lagrangian scheme* based on time series of temperatures at nodes (i.e. intersection points between different components) of the the network. A detailed modeling approach for heating networks is presented in [Köcher, 2000], featuring complex network geometries with loops, non-constant thermodynamical properties of water, and unsteady friction models. The main focus of this work lies on optimal network design. A common trait, which most modeling approaches for DHN share, is the description of energy transport in the distribution network as an advection process. In [van der Heijde et al., 2017b], and [van der Heijde et al., 2017a], the authors analyze this class of models, including an experimental validation. In [Hauschild et al., 2019],

an embedding into the framework of *Port-Hamiltonian systems* is presented, with the aim to provide a mathematically and physically rigorous basis to model *coupling of sectors*. Besides district heating, flow based network models have been proven to pose a suitable approach for problems in other areas, traffic, gas transport, or logistic networks. For an overview of network based modelling we refer to [Ambrosio et al., 2013] and [Bressan et al., 2014].
Explicit high order numerical schemes for general *hyperbolic conservation laws* on networks are discussed in [Borsche and Kall, 2014], and [Borsche, 2016]. The presented numerical methods can easily be applied to the field of district heating. As length scales can vary vastly in district heating networks, a global time step restriction can result in large computational costs. In [Borsche et al.,], *local time stepping* (LTS) schemes for networks are used to circumvent this restriction. More common in the field, however, is the use of classical methods, e.g. explicit or implicit Upwind [Vivian et al., 2018] or a modification of the QUICKEST scheme [Grosswindhager et al., 2011].
As already observed, an accurate numerical simulation is essential if sharp estimates of transport time delays are required. On the other hand, such models tend to be computationally intensive and are often too complex for usage in optimization. The *model predictive control* (MPC) approach in [Sandou et al., 2005] tackles this problem by coupling a full nonlinear forward simulation with a simplified, linear approximation, where the former serves as predictor, and the latter is used as an optimization model. In [Giraud et al., 2017], a similar method is used to solve optimal control problems involving multiple, switchable energy sources, resulting in *mixed integer linear programs* (MILP). A nonlinear, instantaneous control approach for district heating networks with power constraints is presented in [Krug et al., 2019]. An outline of the optimization algorithms, which are a part of the approach we present in this thesis, are presented in [Mohring et al., 2021] and [Linn et al., 2019]. Based on a combination of a nonlinear, and a linearized model as well, it eliminates the internal state variables from the optimization model, hence reducing its dimension. First results obtained with this approach for industrial use cases provided the motivation to investigate the subject more thoroughly in this thesis.
An alternative to linearized models for optimization lies in *model order reduction*, as it is depicted in [Rein et al., 2019a] and [Rein et al., 2019b]. Moment matching is applied to approximate the full, high resolution model by one with significantly fewer degrees of freedom, while preserving the system's essential dynamic behaviour.
In [Mohring et al., 2021] another approach was chosen to keep simulation times short. Temperatures, or more precisely, energy densities are represented by low order polynomials on both, local and temporal inflow boundaries of a pipeline, and followed along characteristics. As long as information is propagated only from the local inflow boundary, the method is similar to [Benonysson et al., 1995]. The resulting differential algebraic equations were integrated by classical collocation [Iserles, 2009] and adaptive time stepping is controlled by Richardson extrapolation [Richardson, 1911].
While all previously mentioned methods are based on physical models involving ordinary or partial differential equations, the authors of [Nielsen et al., 2002] present an approach based on stochastic model predictive control, which has successfully been implemented as an on-line controller.
In the field of numerical mathematics and analysis, several relevant studies have contributed to the optimal control of district heating networks. Gugat et al. ([Gugat, 2016]) focused on the exact boundary controllability of traffic flow, which shares mathematical similarities with our application domain. Their work provides insights into addressing similar challenges. Another significant contribution by Gugat et al. ([Gugat et al., 2015]) involved the analysis of systems of nonlocal conservation laws on networks. Considering that nonlocality poses a considerable challenge in our model, their findings offer valuable perspectives.
Although our hydraulic model differs from the more general isothermal Euler equations, Gu-

gat ([Gugat et al., 2012]) studied the H^2-stabilization of such equations. This research is relevant as our model incorporates non-isothermal aspects. Moreover, Ulbrich ([Ulbrich, 2002]) investigated sensitivity and adjoint calculus for discontinuous solutions of hyperbolic conservation laws. While not directly applicable to systems with algebraic constraints like ours, their study offers insights into sensitivity analysis for more general solutions.
The existence and uniqueness of solutions for nonlocal transport equations were explored by Coron ([Coron et al., 2020]). Although not directly related to our district heating networks, their research on nonlocal equations provides a foundation for understanding similar mathematical properties. Alberto ([Alberto and Andrea, 1995]) developed variational calculus methods for discontinuous solutions of hyperbolic conservation laws, which contributes to the broader understanding of mathematical techniques applicable to our work.
To assess the accuracy of finite volume schemes, Merlet ([Merlet and Vovelle, 2007]) conducted error estimation studies. Their work offers valuable insights into quantifying errors in numerical approximations, which is crucial for our optimization efforts. Additionally, Merlet ([Merlet, 2008]) explored L^∞ and L^2 error estimates for finite volume schemes. These findings further support the evaluation and validation of our numerical approaches.
By incorporating these studies from numerical mathematics and analysis into the optimal control of district heating networks, we can enhance our understanding of the mathematical foundations and refine our numerical methods to improve the overall efficiency and accuracy of our models.
Besides a numerical simulation of the distribution network, a good load prediction is essential for precise numerical simulation and optimization. Here, standardized load profiles [BGW, 2006], which originally have been developed in the context of gas networks, may serve as a good starting point, if no detailed measurements are available.

1.2 The structure of this thesis and main results

This thesis is structured as follows:
We continue in CHAPTER 2 with a detailed derivation of the complete system of governing equations for the network. We start with a short overview of the relevant physical quantities (including a summary of the thermodynamic properties of water) and then introduce the necessary components to set up a graph based network model. The transport equations for water and thermal energy in pipelines are presented in dimensional form as well as in scaled form, with all physical quantities related to characteristic units, and physical process parameters expressed in dimensionless numbers. Further model elements account for fluxes and coupling conditions, and the terms representing consumers and producers. We finish the chapter with a one page summary of the complete model equations.
In CHAPTER 3, which represents the mathematical core of our thesis work, we perform an analysis of the solvability of the model equations, starting from the scalar advection problem in a single–consumer single–producer (SCSP) network, to a generalized problem suitable to model simple networks without loops. Following the SCSP case, we study well-posedness and regularity for networks without flow reversal. We then introduce abstract residual and solution operators on suitable Banach spaces to derive an abstract formulation of the problem, which serves as a rigorous mathematical model that can be utilized for optimization problems.
In CHAPTER 4 we turn towards optimal control problems built upon the model which we have established in CHAPTER 2, and demonstrate their numerical solution by applying the insights from the mathematical analysis of the models carried out in CHAPTER 3. After some brief considerations on the existence of local solutions with regularized state constraints, we explain the algorithmic component of projected gradient descent in H^1, including a short comparison of L^2 to H^1 gradients, followed by an outline on numerical discretization schemes and automatic differentiation utilized to obtain the discrete adjoint and the propagation of sensitivities. Finally we show two application examples: The application of the H^1 projected gradient algorithm to a single pipeline network, and the optimal operation of a real world district heating network using discrete sensitivity propagation.
In CHAPTER 5 we conclude the thesis with a short summary of our results, and give an outlook on further work that could be performed on this basis.

Constributions of this thesis

We finish the introductory chapter with a short list of results that we obtained in our thesis and that to our knowledge extend the state of the art of industrial mathematics applied to district heating network simulation and optimization:

- **Improved DHN modeling:** Adaption of the already existing mathematical models ([Mohring et al., 2021], [Krug et al., 2019]) with focus on a consistent water model, and solvability of the equations independent of the feasibility of state inequality constraints.
- **Extensions in the mathematical analysis of DHN models:** Existence and uniqueness results in C^0, as well as H^1 for district heating networks where flow reversals cannot occur.
- **Weak formulation for optimal control:** Motivated by the solution theory for parabolic equations: Weak formulation in Bochner spaces which permit differentiability and weak-weak* continuity. The first property is necessary to establish optimality conditions for this non-convex system, the second one aids as a theoretical tool to prove existence of local minimizers.
- **Application in a projected gradient method:** H^1 projection is performed by transformation into an obstacle problem, for which established methods exist.

The case studies presented in CHAPTER *4* indicate how these theoretical results can be favourably utilized to perform transient simulations of real world DHN and optimize their performance by optimal control.

Chapter 2

Derivation of the governing equations

In district heating, thermal energy is transported from one (or few) central producers to many distributed consumers via a network of water pipelines. Therefore, the domain of hydraulics and thermodynamics provides the modelling basis to simulate the functionality and physical properties of district heating networks.
An overview of typical quantities of interest, as well as their assumed range of magnitude is given in table TABLE *2.1*.

Symbol	Name	(SI) Unit	Magnitude
p	hydraulic pressure	Pa	$10^5 - 10^6$
v	flow velocity	$m \cdot s^{-1}$	$10^{-2} - 10^0$
ρ	mass density	$kg \cdot m^{-3}$	$\sim 10^3$
e	internal energy density	J $\cdot m^{-3}$	$10^8 - 10^9$
T	temperature	$°C$	$10^1 - 10^2$
q	volumetric flow rate	$m^3 \cdot s^{-1}$	$10^{-4} - 10^{-2}$
$\hat{q}$	mass flow rate	k$g \cdot s^{-1}$	$10^{-1} - 10^1$
Q	energy flow rate / power	W	$10^4 - 10^7$

Table 2.1: Model variables and their typical magnitudes

Mathematical models describing transient, spatial transport processes display the interplay of the involved time and length scales, which are summarized in TABLE *2.2*, and TABLE *2.3*.
While a three dimensional, high resolution numerical model would certainly be nice to have, we need to keep in mind that the model is going to be used in the context of optimization problems covering a time range of multiple days. In order to keep computation times at an acceptable level, we therefore choose a graph based modelling approach for our district heating network. This involves the usage of a simplified, one dimensional pipeline

Symbol	Range	Description
Δx_{net}	1-10 km	Average network diameter
L	0.1-1000 m	Pipeline length
Δx_{sim}	<100m	Desired simulation length scale

Table 2.2: Relevant length scales in district heating

Symbol	Range	Description
Δt_{hyd}	$\leqq$ 1 s	Estimated network traversal time of hydraulic shock waves
Δt_{adv}	$10^0 - 10^4$ s	Average advective pipeline traversal time
Δt_{opt}	15 min	Operational control time interval
Δt_{sim}	1-15 min	Desired numerical simulation time scale

Table 2.3: Relevant time scales in district heating

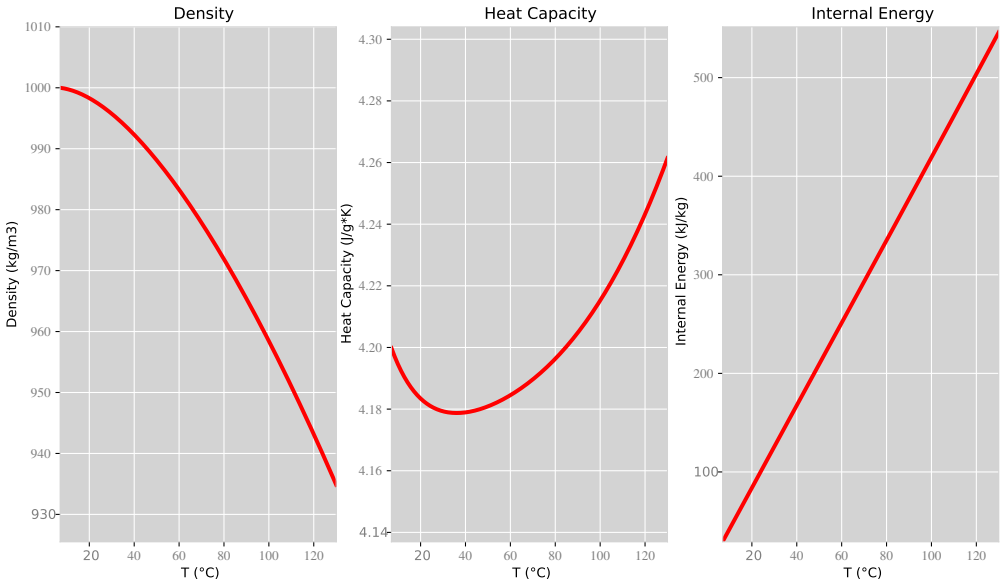

Figure 2.1: Isobaric fluid properties of water at $P = 3.0$ bar, taken from the NIST chemistry webbook [NIST, 2016]

model, whose practical accuracy has been investigated in [van der Heijde et al., 2017b], and [van der Heijde et al., 2017a].
The entire network model is structured into five parts:
An approximate polynomial model for the thermodynamic properties of water is given in section SECTION *2.1*.
In SECTION *2.2*, we introduce a graph based model, which describes the interaction between different components in the form of coupling and boundary conditions. The model equations and constraints for different network components, namely *pipelines*, *producers*, and *consumers*, are established in SECTION *2.3*, SECTION *2.4*, and SECTION *2.5*.

2.1 Thermodynamic Properties of Water

In district heating, one makes use of the good heat storage capacities of water, in order to transport thermal energy over long distances.
Quantities of interest are *temperature* T, *mass density* ρ, the (non-specific) *internal energy density* e, and *heat capacity* c_v. FIGURE *2.1* shows the variation of these quantities in the temperature range *7 °C* $\leq$ *130 °C* at a constant pressure level of *3 bar*.
The relative changes in magnitude given in TABLE *2.4* support the following assumption:

	Density	Internal Energy	Heat Capacity
isothermal	0.052	0.065	0.099
isobaric	6.681	179.987	1.968

Table 2.4: Relative changes (w.r.to mean) of fluid properties in % in isobaric (p = 3.0 bar, 7.0 °C $\leq$ T $\leq$ 130.0 °C) and isothermal (T = 7.0 °C, 3.0 bar $\leq$ p $\leq$ 14.0 bar) settings.

Assumption 2.1

The influence of pressure to internal energy and mass density can be neglected.

For the remaining quantities *temperature* T, the (non-specific) *internal energy density* e, *heat capacity* c_v, and *mass density* ρ, we want to establish a polynomial model, which is inherently consistent. Starting with an approximation of c_v, the *specific density of internal energy* $u(T)$ is given by

$$u(T) = u(T_{min}) + \int_{T_{min}}^{T} c_v(\theta)\, d\theta. \tag{2.1}$$

Therefore, the total amount of internal energy $U(T)$ contained in a volume Ω is given by the integral

$$U(T) = \int_{\Omega} \rho(T)u(T)\, dV = \int_{\Omega} e(T)\, dV, \tag{2.2}$$

where

$$e(T) = \rho(T)u(T) \tag{2.3}$$

denotes the *(internal) energy density per unit volume*. In order to replace the basis variable T by e, the mapping $T \mapsto e(T)$ needs to be bijective within the context of our model. A sufficient condition for this is that the derivative satisfies

$$\frac{de(T)}{dT} > 0 \tag{2.4}$$

for any feasible temperature. Using the definition of u, this leads to the inequality

$$\frac{de(T)}{dT} = \frac{d\rho(T)}{dT}u(T) + \rho(T)c_v(T) > 0. \tag{2.5}$$

The inverted mapping $e \mapsto T(e)$ can be obtained by integrating its derivative

$$\frac{dT}{de} = T'(e) = \frac{1}{e'(T(e))} = \frac{1}{\rho c_v + \rho' e}, \tag{2.6}$$

where $\cdot'$ denotes the derivative of an univariate function w.r.t. its argument. In many applications, only the quantities ρ, e (or u), and T are needed, whereas exact values c_v are not required.

Assumption 2.2: Polynomial thermodynamic model

Given polynomial approximations $\tilde{\rho}$ and $\tilde{c_v}$ and an admissible temperature range $[T_{min}, T_{max}]$, we assume the following:

W.1 $\tilde{\rho}$ and $\tilde{c_v}$ only depend on T, but not on p.

W.2 $\tilde{\rho}$ is bounded, strictly positive, and nowhere increasing .

W.3 $\tilde{c_v}$ is bounded, strictly positive, and convex .

W.4 The mapping $T \mapsto e(T)$ defined in (2.3) is a diffeomorphism from $[T_{min}, T_{max}]$ to $[e_{min}, e_{max}]$. Further, its inverse preserves the properties of $\tilde{\rho}$ and $\tilde{c_v}$ in the sense that $\rho = \tilde{\rho} \circ T(e)$, and $c_v = \tilde{c_v} \circ T(e)$ satisfy **W.2** and **W.3**, respectively.

The values of T in FIGURE *2.1* motivate a *linear* model for u, which implies a *constant* approximation of c_v. Even though the qualitative behaviour depicted in figure FIGURE *2.1* suggests a polynomial approximation of at least second order, the relative deviations given in TABLE *2.4* show, that a mean value approximation of ρ,

$$\bar{\rho} = \frac{1}{T_{max} - T_{min}} \int_{T_{min}}^{T} \rho(\theta)\, d\theta, \tag{2.7}$$

and c_v

$$\bar{c_v} = \frac{1}{T_{max} - T_{min}} \int_{T_{min}}^{T} c_v(\theta)\, d\theta, \tag{2.8}$$

should be sufficient for many practical applications. As we are going to show in SECTION *3.1*, such a simplified constitutive law poses an important special case, for which we can explicitly solve the model equations of the pipeline derived in SECTION *2.3*. Furthermore, conservation of mass and volume are equivalent, when the mass density is assumed to be constant.
The resulting models of the specific internal energy density

$$u(T) = u(T_{min}) + \bar{c}_v\,(T - T_{min}) \tag{2.9}$$

and non-specific internal energy density

$$\begin{aligned} e(T) &= \bar{\rho} u(T_{min}) + \bar{\rho}\bar{c_v}\,(T - T_{min}) \\ &= e_{min} + \bar{\rho}\bar{c_v}\,(T - T_{min})\,, \end{aligned} \tag{2.10}$$

are affine linear functions. We thus can invert (2.10), and obtain an explicit expression

$$T(e) = T_{min} + \frac{e - e_{min}}{\bar{\rho}\bar{c_v}} \tag{2.11}$$

of the temperature T in terms of e, which is affine linear as well. These considerations motivate the following approximations to the material model of ASSUMPTION *2.2*:

Assumption 2.3: Averaged thermodynamic model

W.2' The mass density is approximated by its average $\rho(e) \equiv \bar{\rho}$.

W.3' The specific heat capacity is approximated by its average $c_v(e) \equiv \bar{c_v}$.

W.4' The mapping $e \mapsto T(e)$ is explicitly given by the affine function (2.11).

2.2 Graph Based Network Model

From the macroscopic point of view, the district heating network is modelled as an oriented, finite graph $\mathcal{G} = (\mathcal{N}, \mathcal{A})$, and an injective *adjacency mapping*. A quick summary of basic concepts from graph theory is summarized in DEFINITION 2.4 (for a complete introduction into the topic, see e.g. [Bondy and Murty, 2008]).

2.4 Definition (Basic definitions from graph theory)

An ordered pair $(\mathcal{N}, \mathcal{A})$ *is called* finite, unordered graph*, where the* vertex set $\mathcal{N}$*, and the* edge set $\mathcal{A} \subset \mathcal{N} \times \mathcal{N}$*, which consists of* ordered tuples *of nodes, are both finite. The graph is called simple, if for two nodes* $n_1, n_2 \in \mathcal{N}$ *there exists at most one edge* a *with* $a = (n_1, n_2)$ *or* $a = (n_2, n_1)$ *(i.e. there are no double edges).*
A graph is called oriented*, if there exist mapping*

$$\begin{aligned} \mathcal{A} &\longrightarrow \mathcal{N} \times \mathcal{N} \\ a &\longmapsto (i(a), o(a)) \end{aligned} \tag{2.12}$$

which identify each edge with their incoming $i(a)$*, and* outgoing node $o(a)$*.*
A sequence of nodes $(n_i)_i$ *is called* path*, if* $(n_i, n_{i+1}) \in \mathcal{A}$*. Such a path is called* orientation preserving*, if there exists a sequence of edges, such that* $i(a_i) = n_i$*, and* $o(a_i) = n_{i+1}$*.*
A graph is called connected*, if there exists a path between every pair of distinct nodes. It is called* acyclic*, if there exists at most one connecting path.*
For an oriented graph $(\mathcal{N}, \mathcal{A}, i, o)$*, we define the incidence sets*

$$\begin{aligned} \mathcal{I}(n) &= \left\{ a \in \mathcal{A} \,\middle|\, i(a) = n \vee o(a) = n \right\}, \\ \mathcal{I}^+(n) &= \left\{ a \in \mathcal{A} \,\middle|\, o(a) = n \right\}, \\ \mathcal{I}^-(n) &= \left\{ a \in \mathcal{A} \,\middle|\, i(a) = n \right\}, \end{aligned} \tag{2.13}$$

as well as the signed incidence matrix

$$I_{n,a} = \begin{cases} +1, n = o(a) \\ -1, n = i(a) \\ 0, \textit{else} \end{cases} \qquad a \in \mathcal{A} \tag{2.14}$$

of the network. We now can define the degree *of a node*

$$\textit{deg}(n) = |\mathcal{I}(n)| \tag{2.15}$$

as the size of its incidence set.

Starting from these basic definitions, we may characterize the graph-topological properties of a district heating network (in the following abbreviated by *DHN*) as follows:

Assumption 2.5: Graph topology of district heating networks

Let $\mathfrak{G} = (\mathcal{N}, \mathcal{A})$ be the graph associated with the topology of a district heating network. We assume that the following properties are fulfilled:

G.1 $\mathfrak{G}$ is finite, simple, oriented, and connected.

G.2 The edge set is a disjoint union $\mathcal{A} = \mathcal{A}_P \sqcup \mathcal{A}_C \sqcup \mathcal{A}_S$, where the subsets contain all edges representing pipes $\mathcal{A}_P$, consumers $\mathcal{A}_C$, and producers $\mathcal{A}_S$.

G.3 There are no leaves, i.e. for every node $n \in \mathcal{N}$ it holds that $deg(n) \geq 2$.

G.4 The set of pipes can be further partitioned into its *forward flow* $\mathcal{A}_P^{ff}$, and *return flow* subset $\mathcal{A}_P^{rf}$. The former one is the pipe subnetwork, which transports heated water from the production plants $\mathcal{A}_S$ to the consumers' $\mathcal{A}_C$ water inlets, whereas the later one is the pipe subnetwork, which transports water from the consumers' outlets back to the producers. If we introduce the node sets

$$\mathcal{N}^{ff} = \left\{ n \in \mathcal{N} \,\middle|\, i(a) = n \vee o(a) = n \text{ for some } a \in \mathcal{A}_P^{ff} \right\}, \tag{2.16a}$$

$$\mathcal{N}^{rf} = \left\{ n \in \mathcal{N} \,\middle|\, i(a) = n \vee o(a) = n \text{ for some } a \in \mathcal{A}_P^{rf} \right\}, \tag{2.16b}$$

$$\mathcal{N}^{ext} = \left\{ n \in \mathcal{N} \,\middle|\, i(a) = n \vee o(a) = n \text{ for some } a \in \mathcal{A}_C \cup \mathcal{A}_S \right\}, \tag{2.16c}$$

then the sub graphs $\mathfrak{G}^{ff} = \left(\mathcal{N}^{ff}, \mathcal{A}_P^{ff}\right)$, and $\mathfrak{G}^{rf} = \left(\mathcal{N}^{ff}, \mathcal{A}_P^{rf}\right)$ are connected.

Whereas heating networks with redundant paths (loops) exist, networks with a treelike topology are quite common, as well. They form an interesting special case, which allows to study the interaction of complex, advective systems, without having to deal with non-smooth phenomena, such as flow indirection.

2.6 Definition (Simple district heating networks)

Let $\mathfrak{G} = (\mathcal{N}, \mathcal{A})$ be the graph associated with the topology of a district heating network, which satisfies all assumptions in ASSUMPTION 2.5*. We call the district heating network* simple*, if the following is true:*

G.5 *There is only one producer such that $\mathcal{A}_S = \{s\}$. We define $n^{rf} := i(s)$, and $n^{ff} := o(s)$.*

G.6 *There are no immediate connections from the producer to any consumer: $\mathcal{I}\left(n^{ff}\right) \setminus \{s\} \subset \mathcal{A}_P^{ff}$.*

G.7 *Let $\mathcal{N}_C = \left\{ n \in \mathcal{N} \,\middle|\, \exists c \in \mathcal{A}_C : i(c) = n \right\}$ denote the set of all forward flow nodes attached to a consumer. Then $deg(n) = 2$ and $\mathcal{I}(n) \cap \mathcal{A}_P^{ff} \neq \emptyset \; \forall n \in \mathcal{N}_C$, such that every consumer has a unique supply pipeline.*

G.8 *For each $n \in \mathcal{N}^{ff}$, the path connecting n^{ff} with n is* orientation preserving *(see* DEFINITION 2.4*). In the same way, for each $n \in \mathcal{N}^{rf}$, the path connecting n with n^{rf} is orientation preserving.*

Remark 2.7

With the assumptions of DEFINITION 2.6, it follows immediately that the sub graphs $\mathfrak{G}^{ff}$ is a tree with root node n^{ff}, and $\mathfrak{G}^{rf}$ is an inverted tree with root node n^{rf}.

2.2.1 Fluxes and coupling conditions

In the following, we assume that all edges and nodes are part of a simple district heating network in the sense of definition DEFINITION 2.6, unless stated otherwise. For each edge, we introduce the following notation for the set of fluxes directed towards their incident nodes, where we denote volume fluxes by q, mass fluxes by $\hat{q}$, and energy fluxes by Q. To be more specific, consider the pair of mass fluxes $\hat{q}_{a:in}, \hat{q}_{a:out}$ of a with respect to its adjacent nodes. We introduce the notation

$$\hat{q}_{a:n} = \begin{cases} \hat{q}_{a:in}, & i(a) = n \\ \hat{q}_{a:out}, & o(a) = n \end{cases} \tag{2.17}$$

such that $\hat{q}_{a:n} > 0$ when mass is moving out of the edge in direction of the node n, and $\hat{q}_{a:n} < 0$ if mass is transported into the edge.
In the same way, we define volume $q_{a:n}$, and (heat) energy fluxes $Q_{a:n}$. We do not assign any volume to nodes, such that they cannot store quantities of any kind. The principle of *total mass conservation* therefore translates to

$$\sum_{a \in \mathcal{I}(n)} \hat{q}_{a:n} = 0 \tag{2.18}$$

whereas *heat energy conservation* requires that

$$\sum_{a \in \mathcal{I}(n)} Q_{a:n} = 0 \tag{2.19}$$

holds true for all nodes.

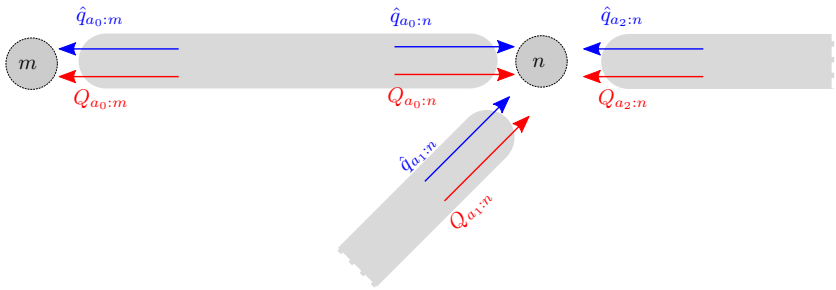

Figure 2.2: Definition of pipeline fluxes

Next, we want to make sure that the fluxes and their coupling conditions are compatible with the material law established in SECTION 2.1. For this purpose, we assume that the expression $e_{a:n}$ is well defined for each edge, where its exact meaning is given in the upcoming SECTION 2.3, and SECTION 2.5. We define the mass and energy fluxes through the relations

$$\hat{q}_{a:n} = \rho(e_{a:n}) q_{a:n}, \tag{2.20a}$$
$$Q_{a:n} = e_{a:n} q_{a:n}, \tag{2.20b}$$

such that it is only necessary to know either $\hat{q}$, or q. In the special case, that $deg(n) = 2$, one easily sees that

$$e_{a1:n} = e_{a2:n} \tag{2.21}$$

is the only possible solution. In general, the conservation laws alone leave the system undetermined, such that one needs to add additional conditions. A common choice is the *perfect mixing assumption*, which requires that

$$Q_{a:n} = e_n q_{a:n} \, \forall a \in \mathcal{I}(n) : q_{a:n} < 0, \tag{2.22}$$

or in terms of energy densities,

$$e_{a:n} = e_n \, \forall a \in \mathcal{I}(n) : q_{a:n} < 0, \tag{2.23}$$

where e_n is the (implicitly) defined *mixing energy* of the node n. We will later see in section 2.3, that this is compatible with the boundary conditions of transport models for pipelines. In the same way, we assume that the expression $p_{a:n}$ is well defined for each edge. Anticipating section 2.3, we require that pressure is continuous across junctions, such that

$$p_{a:n} = p_n \, \forall a \in \mathcal{I}(n). \tag{2.24}$$

This completes the treatment of coupling conditions between different components, and we proceed with derivation of model equations describing the behaviour of pipelines, consumers, and producers.

2.3 Hydrodynamic and Thermal Energy Transport in Pipelines

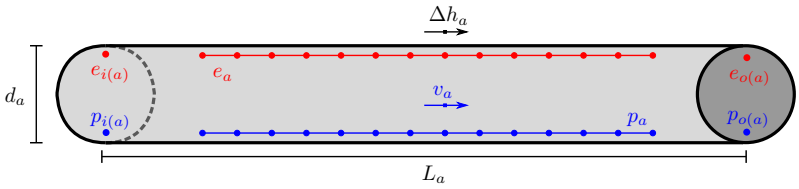

Figure 2.3: Variables and parameters of a pipeline a

In this section we consider a single pipeline with length L, and diameter d, as depicted in FIGURE 2.3 (here with subscript a). We want to model the evolution of *flow velocity* v, *hydraulic pressure* p, and *energy density* e, both in space and time. The starting point for our pipeline model are the one dimensional Euler equations for a thermodynamic system (see e.g. [LeVeque, 2008])

$$\partial_t \rho + \partial_x (\rho v) = 0, \tag{2.25a}$$
$$\partial_t (\rho v) + \partial_x \left(\rho(v^2 + gh) + p\right) = 0, \tag{2.25b}$$
$$\partial_t E + \partial_x (v(E + p)) = 0, \tag{2.25c}$$

where

$$E = \frac{1}{2}\rho v^2 + \rho g h + e \tag{2.26}$$

is the total energy of the system. Besides the advection driven transport of energy, the equations (2.25) also describe physical effects, such as the propagation of hydraulic pressure waves, which are hard to resolve at the desired length and time scales (see TABLE 2.2 ,

and TABLE 2.3), and only of lesser interest in water driven district heating. Due to the large number of pipelines in a DHN, and the need to repeatedly solve the model equations in the context of optimization, we wish to further simplify (2.25), to obtain a model which is better suited for this use case. We introduce the *convective derivative*

$$\frac{Df}{Dt} = \partial_t f + v\partial_x f \tag{2.27}$$

and reformulate (2.25) to

$$\frac{D\rho}{Dt} = -\rho\partial_x v \tag{2.28a}$$

$$\frac{Dv}{Dt} = -\frac{\partial_x p}{\rho} + gh_x - \underbrace{\frac{v\,|v|}{2d}\lambda}_{f_{frict}} \tag{2.28b}$$

$$\frac{De}{Dt} = -\left(e+p\right)\partial_x v - \underbrace{\frac{4k}{d}\left(T - T_{wall}\right)}_{f_{loss}} - \underbrace{\partial_x\left(D_w\partial_x T\right)}_{f_{diff}} \tag{2.28c}$$

where the terms f_{frict}, f_{loss}, and f_{diff} are additional source (or reaction) terms modelling pressure loss due to friction, energy loss through conduction, and diffusive energy transport, respectively. To be more precise, the influence of friction is modelled by

$$f_{frict} = -\frac{v\,|v|}{2d}\lambda \tag{2.29}$$

which depends on the dimensionless *friction factor* λ, which we are going to treat as an unknown parameter for now. The energy loss term

$$f_{loss} = \frac{4k}{d}\left(T - T_{wall}\right) \tag{2.30}$$

is obtained by integrating the heat flux according to Fourier's law around the pipe's diameter, with k being the *heat transmission coefficient*. The final term

$$f_{diff} = \partial_x\left(D_w\partial_x T\right) \tag{2.31}$$

models the transport of energy by diffusion, where D_w is the thermal conductivity of water. From section 2.1, we know that T follows the differential rule

$$\frac{dT}{de} = \frac{\rho}{\rho' e + \rho^2 c_v} \tag{2.32}$$

such that the diffusion term expands to

$$\begin{aligned}\partial_x\left(D_w\partial_x T\right) &= \partial_x\left(D_w\frac{\rho}{\rho' e + \rho^2 c_v}\partial_x e\right)\\ &= \partial_x\left(D_w\frac{\rho}{\rho' e + \rho^2 c_v}\right)\partial_x e + D_w\frac{\rho}{\rho' e + \rho^2 c_v}\partial_{xx} e.\end{aligned} \tag{2.33}$$

According to the model scales given in TABLE 2.1, this expression can be roughly approximated by the linear diffusion term

$$\partial_x\left(D_w\partial_x T\right) \approx \varepsilon\partial_{xx} e, \tag{2.34}$$

where we define the *averaged diffusion parameter* as

$$\varepsilon = D_w\frac{1}{\bar{\rho}\bar{c_v}}. \tag{2.35}$$

Using the values given in TABLE 2.1, its magnitude can be estimated by $\varepsilon \approx 10^{-6}\frac{m^2}{s}$. Plugging this simplification into our model equations (2.28), we end up with

$$\frac{D\rho}{Dt} = -\rho\partial_x v, \tag{2.36a}$$
$$\frac{Dv}{Dt} = -\frac{\partial_x p}{\rho} + gh_x - \frac{v\,|v|}{2d}\lambda, \tag{2.36b}$$
$$\frac{De}{Dt} = -\left(p+e\right)\partial_x v - \frac{4k}{d}\left(T - T_{wall}\right) - \varepsilon\partial_{xx}e. \tag{2.36c}$$

Next, we want to estimate the importance of each reaming term in the model, in order to simplify it even further. For this purpose we introduce reference scales according to TABLE 2.3, TABLE 2.2, and TABLE 2.1, as well as *dimensionless scaled quantities*

$$\begin{aligned} \tilde{x} &= \frac{x}{x_{ref}}, & \tilde{t} &= \frac{t}{t_{ref}}, & \tilde{h} &= \frac{h}{h_{ref}} \\ \tilde{v} &= \frac{v}{v_{ref}}, & \tilde{e} &= \frac{e}{e_{ref}}, & \tilde{p} &= \frac{p}{p_{ref}}, \\ & & \tilde{\rho} &= \frac{\rho}{\rho_{ref}}, & \tilde{T} &= \frac{T}{T_{ref}}, \end{aligned} \tag{2.37}$$

together with a set of *dimensionless numbers*

$$\begin{aligned} c &= \frac{t_{ref}v_{ref}}{x_{ref}} && \text{(reference CFL number)}, \\ m &= \sqrt{\frac{\rho_{ref}v_{ref}^2}{p_{ref}}} && \text{(Mach's number)}, \\ \delta &= \frac{d}{x_{ref}} && \text{(relative diameter)}, \\ \kappa &= \frac{4k}{d}\frac{t_{ref}T_{ref}}{e_{ref}} && \text{(energy transmission number)}, \\ Fr &= \sqrt{\frac{gh_{ref}}{v_{ref}^2}} && \text{(Froude number)}, \\ Pe &= \frac{cx_{ref}^2}{t_{ref}\varepsilon} && \text{(Peclet number)}, \end{aligned} \tag{2.38}$$

and obtain a set of *scaled equations*

$$\frac{D\tilde{\rho}}{D\tilde{t}} = -c\tilde{\rho}\partial_{\tilde{x}}\tilde{v}, \tag{2.39a}$$
$$\frac{1}{c}\frac{D\tilde{v}}{D\tilde{t}} = -\frac{1}{m^2}\frac{\partial_{\tilde{x}}\tilde{p}}{\tilde{\rho}} - \frac{1}{Fr^2}\partial_{\tilde{x}}\tilde{h} - \frac{\lambda}{2\delta}\tilde{v}\,|\tilde{v}|\,, \tag{2.39b}$$
$$\frac{D\tilde{e}}{D\tilde{t}} = -\left(\tilde{e} + \frac{p_{ref}}{e_{ref}}\tilde{p}\right)c\partial_{\tilde{x}}\tilde{v} - \kappa\left(\tilde{T} - \tilde{T}_{wall}\right) - \frac{1}{Pe}\partial_{\tilde{x}\tilde{x}}\tilde{e}, \tag{2.39c}$$

which allow us to compare the impact of different terms to each equation. Due to the small magnitude of the diffusion parameter ε, we wish to compare it against the advective transport and loss terms. Comparing the respective scaling factors, we can see that the estimates

$$cPe = \frac{c^2x_{ref}^2}{\varepsilon t_{ref}} \gg 1, \tag{2.40}$$

and

$$\kappa Pe = 4\frac{k}{d}\frac{T_{ref}}{e_{ref}}\frac{cx_{ref}^2}{\varepsilon} \gg 1, \tag{2.41}$$

hold, if the magnitude of the flow velocity v has a positive lower bound $|v| \geq v^{min} > 0$. In this case, diffusive effects are dominated by advection and cooling, such that we can safely dismiss them, and we continue with the slightly simplified system

$$\frac{D\tilde{\rho}}{D\tilde{t}} = -c\tilde{\rho}\partial_{\tilde{x}}\tilde{v}, \tag{2.42a}$$

$$\frac{1}{c}\frac{D\tilde{v}}{D\tilde{t}} = -\frac{1}{m^2}\frac{\partial_{\tilde{x}}\tilde{p}}{\tilde{\rho}} - \frac{1}{Fr^2}\partial_{\tilde{x}}\tilde{h} - \frac{\lambda}{2\delta}\tilde{v}\left|\tilde{v}\right|, \tag{2.42b}$$

$$\frac{D\tilde{e}}{D\tilde{t}} = -\left(\tilde{e} + \frac{p_{ref}}{e_{ref}}\tilde{p}\right)c\partial_{\tilde{x}}\tilde{v} - \kappa\left(\tilde{T} - \tilde{T}_{wall}\right). \tag{2.42c}$$

2.3.1 Incompressible model

In SECTION 2.1 we have established a constitutive law for water, which defines the quantities ρ, c_v, and T as functions of the internal energy density e. In particular, these quantities do not depend on the hydraulic pressure. Therefore, any variation of ρ is the consequence of a variation of e caused by (de-)compression and cooling. We are going to show, that these influences are negligible for our use case. In order to do so, we make the assumption, that the density is constant along *characteristics* (see SECTION 3.1.1 for a discussion of this term)

$$\frac{D\rho}{Dt} = 0, \tag{2.43}$$

which directly leads to

$$\partial_x v = 0, \tag{2.44}$$

resulting in the simplified, incompressible model

$$\partial_{\tilde{x}}\tilde{v} = 0, \tag{2.45a}$$

$$\frac{1}{m^2}\partial_{\tilde{x}}\tilde{p} = -\frac{1}{c}\tilde{\rho}\partial_{\tilde{t}}\tilde{v} - \frac{\tilde{v}\left|\tilde{v}\right|}{2\delta}\tilde{\rho}\lambda - \tilde{\rho}\frac{1}{Fr^2}\partial_{\tilde{x}}\tilde{h}, \tag{2.45b}$$

$$\frac{D\tilde{e}}{D\tilde{t}} = -\kappa\left(\tilde{T} - \tilde{T}_{wall}\right). \tag{2.45c}$$

Due to the constitutive law $\rho = \rho(e)$ the continuity equation then becomes

$$\rho'\frac{D}{Dt}e = 0, \tag{2.46}$$

which is fulfilled, either if $\tilde{\rho}' = 0$, or $\frac{D}{Dt}\tilde{e} = 0$. The first case is applicable whenever a constant material law for the water density is chosen, then second one requires the absence of diffusive effects and conductive energy loss. If neither of these conditions is satisfied, the incompressibility assumption introduces a model error. By combining (2.45) with the material laws from section 2.1

$$\begin{aligned} -c\tilde{\rho}\partial_{\tilde{x}} &= \frac{D\tilde{\rho}}{D\tilde{t}} \\ &= \tilde{\rho}'\frac{D\tilde{e}}{D\tilde{t}} \\ &= -\tilde{\rho}'\left(\tilde{e} + \frac{p_{ref}}{e_{ref}}\tilde{p}\right)c\partial_{\tilde{x}}\tilde{v} - \kappa\left(\tilde{T} - \tilde{T}_{wall}\right). \end{aligned} \tag{2.47}$$

we obtain

$$\partial_{\tilde{x}}\tilde{v} = \frac{\tilde{\rho}'}{\tilde{\rho}} \frac{1}{1 - \frac{\tilde{\rho}'}{\tilde{\rho}}\left(\tilde{e} + \frac{p_{ref}}{e_{ref}}\tilde{p}\right)} \frac{\kappa}{c}\left(\tilde{T} - \tilde{T}_{wall}\right) \tag{2.48}$$

leading to the estimate

$$\|\partial_{\tilde{x}}\tilde{v}\|_\infty \leq \left\|\frac{\tilde{\rho}'}{\tilde{\rho}}\right\|_\infty \frac{\kappa}{2c}\left(\left\|\tilde{T}\right\|_\infty - \tilde{T}_{wall}\right) \tag{2.49}$$

such that the model error is negligible, as long as the reference CFL number c is relatively large when compared to the cooling term, or the maximal relative change $\left\|\frac{\tilde{\rho}'}{\tilde{\rho}}\right\|_\infty$ of ρ w.r.t. e is comparably small.
Finally, we move back to unscaled variables, and assume a constant slope

$$h_x = \frac{\Delta h}{L}, \tag{2.50}$$

yielding the system of equations

$$\partial_x v = 0 \tag{2.51a}$$

$$\partial_x p = -\frac{v\,|v|}{2d}\rho\lambda - \rho g\frac{\Delta h}{L} \tag{2.51b}$$

$$\partial_t e + v\partial_x e = -\frac{4k}{d}\left(T(e) - T_{wall}\right) \tag{2.51c}$$

which we are going to use as our pipeline model in the upcoming sections.

2.3.2 Pressure losses due to friction

So far, the friction coefficient λ only appeared as a dimensionless parameter, which has yet to be specified.
A common choice is the phenomenological *Colebrook-White* equation ([Moody, 1944])

$$\frac{1}{\sqrt{\lambda}} = -2\log_{10}\left(\frac{\kappa}{3.7d} + \frac{2.51}{\mathrm{Re}\sqrt{\lambda}}\right) \tag{2.52}$$

which depends on the surface roughness κ, and the dimensionless *Reynold's number*

$$Re = \frac{d_{ref}v}{\nu}. \tag{2.53}$$

In general, the *kinematic viscosity* ν changes with temperature (here: e), such that the implicitly defined friction factor has a (point wise) representation $\lambda(t,x) = f_\lambda(e(t,x), v(t))$ (an efficient numerical method is presented in [Clamond, 2009]). In the turbulent limit (i.e. if Re is large), the term involving the Reynold's number becomes negligible, and the simplified equation

$$\frac{1}{\sqrt{\lambda}} = -2\log_{10}\left(\frac{\kappa}{3.7d}\right) \tag{2.54}$$

would pose a good approximation to (2.52). Examining possible values of Re (as shown in FIGURE 2.4) we observe that the flow stays in the fully turbulent regime, as long as v is bounded from below by a sufficiently large, positive constant.
As a result, we define

$$\lambda = \log_{10}\left(\frac{\kappa}{3.7d}\right), \tag{2.55}$$

and from now on treat it as a constant, known parameter for each pipeline.

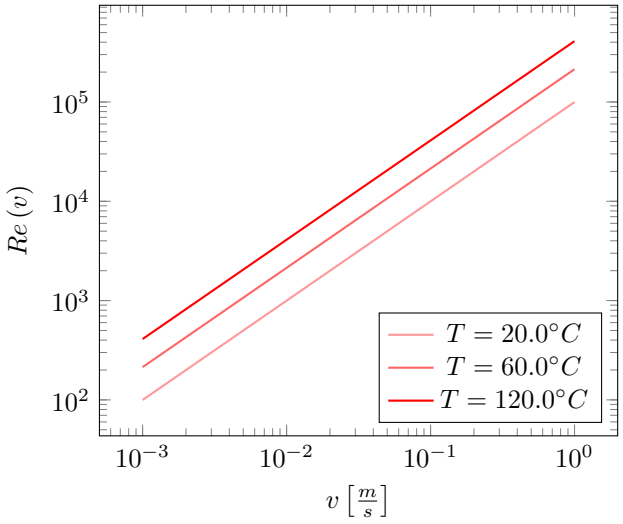

Figure 2.4: Reynolds number for a pipe with d = 0.1 m (data for ν obtained from [NIST, 2016])

2.3.3 Complete pipeline model and boundary conditions

We model the transport of energy in pipeline as a thermohydraulic system, whose state is determined by its spatial energy density e_a, flow velocity v_a, and hydraulic pressure p_a. For each pipe $a \in \mathcal{A}_P$, the state variables are defined as the solutions of a system of partial differential equations

$$\partial_x v_a = 0 \tag{2.56a}$$

$$\partial_t e_a + \partial_x \left(v_a e_a\right) = \underbrace{-\frac{4k_a}{d_a}\left(T\left(e_a\right) - T_a^{wall}\right)}_{-r_a(e_a)} \tag{2.56b}$$

$$\partial_x p = -\rho\left(e_a\right)\left(\frac{\lambda_a}{2d_a} v_a \left|v_a\right| + g\frac{\Delta h_a}{L_a}\right) \tag{2.56c}$$

in the space-time domain $I_t \times \Omega_a = I_t \times [0, L_a]$, together with boundary conditions for p_a, and e_a

$$e_{a:in} = e_{i(a)} \tag{2.57a}$$

$$p_{a:in} = p_{i(a)} \tag{2.57b}$$

$$p_{a:out} = p_{o(a)} \tag{2.57c}$$

as well as an initial condition

$$e_a(t_0, \cdot) = e_a^{init} \tag{2.58}$$

for e_a. Under the assumption that e and p are at least continuous, we *formally* define their *traces* as

$$e_{a:in} = \lim_{x \searrow 0} e_a(\cdot, x), \qquad e_{a:out} = \lim_{x \nearrow L_a} e_a(\cdot, x), \tag{2.59a}$$

$$p_{a:in} = \lim_{x \searrow 0} p_a(\cdot, x), \qquad p_{a:out} = \lim_{x \nearrow L_a} p_a(\cdot, x). \tag{2.59b}$$

(2.59c)

According to our assumptions, the right hand side of (2.56c) does not change its sign in any spatial direction at any fixed time, such that $p(t,x)$ is always monotonous in x. If only the values of the nodal pressures are of interest, we can integrate (2.56c) over the interval $\Omega_a = [0, L_a]$ and obtain

$$p_{o(a)} = p_{i(a)} - \int_{\Omega_a} \rho\left(e_a\right) \left(\frac{\lambda_a}{2d_a} v_a \left|v_a\right| + g \frac{\Delta h_a}{L_a} \right) dx, \tag{2.60}$$

which does not depend on p_a any more.

Remark 2.8: Formal set of equations considering flow indirections

Formally, the inflow boundary conditions can be generalized to

$$\frac{1}{2}\left(v_a + \left|v_a\right|\right)\left(e_{a:in} - e_{i(a)}\right) + \frac{1}{2}\left(v_a - \left|v_a\right|\right)\left(e_{a:out} - e_{o(a)}\right) = 0 \tag{2.61}$$

which is well defined in terms of conservation laws, if v_a is regular enough.

In consistency with the definitions in section 2.2, we define the fluxes

$$q_{a:in} = -v_a A_a, \tag{2.62a}$$
$$q_{a:out} = v_a A_a, \tag{2.62b}$$
$$Q_{a:in} = q_{a:in} e_{a:in}, \tag{2.62c}$$
$$Q_{a:out} = q_{a:out} e_{a:out}. \tag{2.62d}$$

2.4 Consumers

Typically, the consumers' water circuit is separated from the district heating network, and heat energy is transferred via a heat exchanger. Assuming a large enough pressure gradient, the systems mass flow is regulated in such a way, that the hot water fed into the return network has a fixed temperature T_c^{ret}.
Since these processes usually happen on a much smaller time scale, when compared to the delivery network's dynamics, we consider the following simplified, algebraic model for each consumer:

$$\rho\left(e_{i(c)}\right) q_{c:in} + \rho\left(e_c^{ret}\right) q_{c:out} = 0, \tag{2.63a}$$
$$Q_{c:in} - e_{i(c)} q_{c:in} = 0, \tag{2.63b}$$
$$Q_{c:out} - e_c^{ret} q_{c:out} = 0, \tag{2.63c}$$
$$Q_{c:in} + Q_{c:out} + \Delta Q_c^{pred} = 0. \tag{2.63d}$$

In this system, the first and fourth equation are conservation laws for mass and energy, whereas the second and third equation specify the incoming and outgoing energy fluxes in terms of other state variables, and boundary conditions. The *return flow energy* e_c^{ret} is assumed to be constant for each consumer, and implicitly defined as

$$T\left(e_c^{ret}\right) = T_c^{ret}. \tag{2.64}$$

The second boundary condition ΔQ_c^{pred} is the time dependent consumer demand function, which is usually based on historical data, or a prediction model.

Remark 2.9: Choice of q instead of $\hat{q}$ as independent variable

Alternatively, one could choose the *mass fluxes* $\hat{q}_{in}, \hat{q}_{out}$ as independent variables, which would result in the system of equations

$$\hat{q}_{in} + \hat{q}_{out} = 0 \tag{2.65a}$$

$$Q_{in} - \frac{e_{in}}{\rho\left(e_{in}\right)}\hat{q}_{in} = 0 \tag{2.65b}$$

$$Q_{out} - \frac{e_{ret}}{\rho\left(e_{ret}\right)}\hat{q}_{out} = 0 \tag{2.65c}$$

which is algebraically equivalent to (2.63). However, multiplication is easier to deal with than division, which is why we don't consider this option.

Even though we have chosen a simplified, algebraic model over a more detailed one, which models the consumer station's internal state, we have to pay more attention to the consumption prediction model, as it directly affects the district heating network's dynamical behaviour. The derivation and discussion of such a model is covered in SECTION *2.4.1*.
In order to be physically consistent, these algebraic equations have to be complemented with a set of box constraints

$$e_c^{ret} < e^{min} \leq e_{i(c)} \leq e^{max} \tag{2.66}$$

for the supplied energy density $e_i(c)$.
For the same reason, we have to impose constraints on the hydraulic variables

$$p^{min} \leq p_{i(c)} \leq p^{max}, \tag{2.67a}$$

$$\Delta p_c^{min} \leq p_{i(c)} - p_{o(c)} \leq \Delta p_c^{max}, \tag{2.67b}$$

where we allow the bounds for the pressure difference to be set individually for each consumer.

2.4.1 Consumption profiles

We assume, that the consumption prediction model takes the general form

$$\Delta Q_c^{pred}(t) = \Delta Q_c^{avg} \cdot S_c(t) \cdot F_c^{corr} \tag{2.68}$$

where the average consumption ΔQ_c^{avg} (usually given in kWh/d, which technically translates to a unit of power) is a real, positive parameter, which is distinctly defined for each consumer, and the factor F_k^{corr} depends on the air temperature and week day. The dimensionless distribution (or shape) function $S_c(t)$ is assumed to be continuous and normalized, such that

$$\int_{I_t} S_c(t)\, dt = 1, \qquad |I_t| = 24\, h \tag{2.69}$$

whenever the time interval covers an entire day, and the dimensionless correction factor F_c^{corr} accounts for fundamental changes of the consumption behaviour on different weekdays and air temperatures, where the later are assumed to be constant throughout a day.
In general, we expect S_c to depend on the (predicted) average air temperature, and the consumer's *category* (e.g. one family house, apartment building, school, etc.), such that a single shape function is likely to be used for multiple individual consumption models.
A fitting method, which computes consumer shape functions S_c from a combination of numerical simulation and observed net consumption data is described in [Mohring et al., 2021].

However, this method requires observation data of a certain quality and quantity, which might not be available in some cases.
That is why, within this work, we choose another approach, which is based on the *standardized consumption profiles for gas networks* (c.f. [BGW, 2006]), which are widely adopted by many DHN operators. In order to adapt this method to our purposes, we consider a time interval $\left[t^{(k)}, t^{(k+1)}\right)$, which spans exactly one hour, and assume that the daily mean air temperature T^{air} is known. Then, the standardized profiles provide us with hourly averages

$$\int_{t^{(k)}}^{t^{(k+1)}} S(t)\,dt = S_c^{(k)}(T^{air}), \qquad k = 0, \dots, N_t - 1, \tag{2.70}$$

of the distribution function, which are normalized in the sense that

$$\sum_{k=0}^{N_t(=24)} S_c^{(k)}(T^{air}) = 1. \tag{2.71}$$

The correction factor is further split up into

$$F_c^{corr} = F_{c,k}^{day} \cdot h(T^{air}), \tag{2.72}$$

where the factor $F_c^{day,(k)}$ depends on the weekday, and the function h is defined as

$$h(T) = \frac{A}{1 + (\frac{B}{T - T_0})^C} + D + \max \begin{cases} m_H \cdot T + b_H \\ m_W \cdot T + b_W \end{cases}, \; h(8°\text{C}) = 1 \tag{2.73}$$

with parameters $A, B, C, D, m_H, b_H, m_W, b_W$ depending on the consumer category.
In some cases, one chooses

$$\bar{T}^{air} = \frac{\sum_{i=0}^{n} 2^{-i} \cdot T^{air,(-i)}}{\sum_{i=0}^{n} 2^{-i}}, \tag{2.74}$$

as the reference temperature to account for the *thermal inertia* of buildings.
The last missing piece of our continuous consumption profile is the reconstruction of the density function S_c.
In the case of a piecewise linear approximation, one additional boundary condition is needed to make the linear system (2.70) uniquely solvable. Natural boundary conditions

$$S(t^{(N_t-1)}) = S(t^{(N_t)}), \text{ or } \quad S(t^{(1)}) = S(t^{(0)}) \tag{2.75}$$

on either side of the time domain are suitable choices. A realisation of this piecewise linear (P1) reconstruction is shown in the left picture of FIGURE 2.5. This reveals an immediate drawback of this method: The density function oscillates heavily in some regions, and attains values substantially smaller than zero. An alternative approach, which tries to minimize the total variation of S_c instead of providing fixed boundary condition (right picture) , produces better results, but still has too many flaws to be usable. The total variation diminishing piecewise polynomial reconstruction from averages plays an important role in many numerical methods for hyperbolic conservation laws (see e.g. [Shu, 2020] for an overview), and its realizability when including additional constraints is a delicate topic by itself.
A thorough analysis of this problem would be beyond the scope of this thesis, which is why we decided to choose a hands-on approach: Given piecewise averages of the (yet unknown) density S_c, we define the cumulative distribution function C_c as

$$C_c(t) = \int_{t^0}^{t} S(\tilde{t})d\tilde{t} = \Delta t \sum_{k=0}^{\hat{k}-1} F_c^k + \left(t - t^{\hat{k}}\right) F_c^{\hat{k}}, \qquad \hat{k} = \left\lfloor \frac{t}{\Delta t} \right\rfloor, \tag{2.76}$$

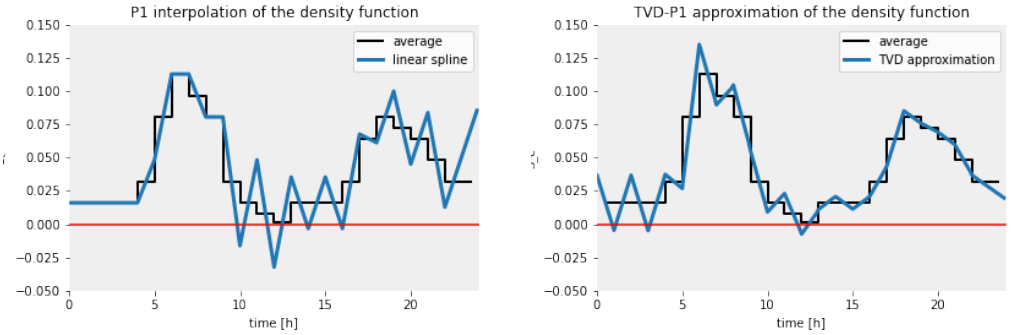

Figure 2.5: P1 interpolation and total variation diminishing (TVD) P1 approximation of S_c

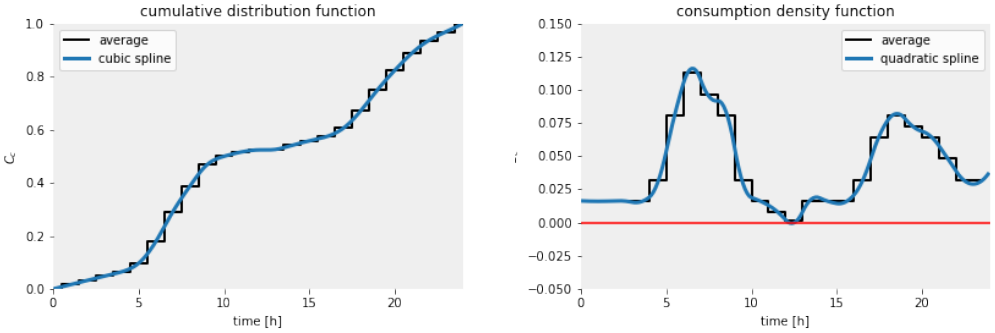

Figure 2.6: Cumulative distribution function (left) and density function (right), as well as their continuous reconstructions

which is piecewise linear, and hence continuous. Knowing of its total variation diminishing properties, we chose cubic polynomial splines to approximate C_c. The density function is retrieved as the derivative $S_c(t) = C_c'(t)$, and therefore is a continuous, piecewise quadratic function. An example of both C_c and S_c is illustrated in FIGURE 2.6.

In some cases it can happen, that the resulting function attains values lower than 0. In order to fix this, we choose an artificial lower bound $S^{min} \geq 0$, and transform the shape function according to

$$\tilde{S}(t) = \max\left(S^{min}, S(t)\right). \tag{2.77}$$

So far, we have constructed a continuous extension of the consumption distribution from piecewise averages. During the interpolation and bounding procedures, the normalization property (2.71) is most likely not preserved. In order to fix this, we consider another normalization step

$$\hat{S}(t) = \frac{\tilde{S}(t)}{\frac{1}{N_{days}} \int_{t^0}^{t^{N_t}} \tilde{S}(t)\, dt}. \tag{2.78}$$

As a consequence of interpolation errors, and the additional renormalization step, the continuous reconstruction $\hat{S}_c$ possibly does not fulfil the interpolation conditions (2.70) exactly. In practise, this deviation has shown to be negligible.

Finally, we consider the case, when the time interval spans multiple days $I_t = \bigcup_{l=0}^{N_{days}-1} I_t^{(l)}$. We can identically apply the reconstruction procedure from above, but have to change the

normalization step to

$$\hat{S}(t) = \frac{\tilde{S}(t)}{\frac{1}{N_{days}} \int_{t^0}^{t^{N_t}} \tilde{S}(t)\, dt}. \tag{2.79}$$

The complete consumption prediction model for a consumer $c \in \mathcal{A}_C$ now reads

$$\Delta Q_c^{pred}(t) = \Delta Q_c^{avg} \sum_{l=0}^{N_{days}-1} F_c^{corr,(l)} S_c(t) \chi_{I_t^{(l)}}(t), \tag{2.80}$$

where $\chi_{I_t^{(l)}}$ is the characteristic functions of the l^{th} time subdomain.

2.4.2 Relaxed model for infeasible supply temperatures

The consumer model (2.63) has to be paired with a set of inequality constraints in order to be complete. In particular, we want to ensure, that the outward oriented volume flux $q_{c:in}$ is always negative (i.e. water flows towards the consumer), which requires that $e_{i(c)} > e_c^{ret}$. In numerical simulations, non-linear systems are commonly solved using iterative methods, where intermediate states usually do not comply with the constraints (2.66)-(2.67). Therefore, we would prefer a more robust set of equations, which preserve the signs of the fluxes. We approach this problem by replacing the supplied energy $e_i(c)$ by the expression

$$\phi_c^{max}\left(e_{i(c)}\right) = \max\left\{e_{i(c)}, e^{min}\right\}. \tag{2.81}$$

This relaxation alters the energy balance equation, such that conservation of thermal energy is no longer maintained, if the energy variable violates the constraint (2.66). As a consequence, the consumer behaviour is not changed whenever (2.66) is satisfied, but the possible maximal volume flow (i.e. velocity) is increased. If a smooth consumer model is preferred, the function ϕ^{max} can be replaced by the piecewise expression

$$\phi_c^{cub}(e) = \begin{cases} e^{min}, & e \leq e^{min} \\ \phi_1(e), & e^{min} < e < e^{crit} \\ e, & e_c^{crit} \leq e \end{cases} \tag{2.82}$$

where $\phi_c^{hermite}$ is the cubic Hermite polynomial satisfying the conditions

$$\phi_1\left(e^{min}\right) = e^{min}, \tag{2.83}$$
$$\phi_1'\left(e^{min}\right) = 0, \tag{2.84}$$
$$\phi_1\left(e_c^{crit}\right) = e_c^{crit}, \tag{2.85}$$
$$\phi_1'\left(e^{crit}\right) = 1. \tag{2.86}$$

Here we introduced an additional parameter e_c^{crit}, which should be chosen within the range

$$e_c^{ret} < e_c^{crit} \leq e^{min}. \tag{2.87}$$

With either approach, the consumers may be as if the supplied temperature was higher than it actually is, resulting in an effective upper bound for the volume fluxes and flow velocities.

2.5 Producers

District heating plants make use of the combined heat output of electricity generators, water boilers, hot water storage tanks, and external sources of thermal energy, such as garbage incineration plants. As such, they usually operate on a much smaller time scale than the hot water supply networks. Therefore, the internal systems of such a heating plant can be quite complex, and usually operate on a much smaller time scale (typically less than a second) than the heating network itself.
In this work, we are primarily focused in the network's capabilities as a thermal energy storage, and the interplay between slowly travelling energy packages, and fast propagating hydraulic consumer response. We assume, that the heating plants control mechanisms are able to track sufficiently smooth reference curve for inflow energy, pressure difference, and reference pressure level, as long as they satisfy a certain set of constraints.
We propose an algebraic model for a *generalized producer*

$$Q_{s:in} = e_{i(s)} q_{s:in} \tag{2.88a}$$
$$Q_{s:out} = u_s^e q_{s:out} \tag{2.88b}$$

where the outgoing energy flux is *partially* determined by the control input u^e.
In the same way, we introduce equations for the hydraulic control variables

$$p_{i(s)} - p_{o(s)} + u_s^{\Delta p} = 0 \tag{2.89a}$$
$$p_{i(s)} = u^{p_0} \tag{2.89b}$$

which involve control inputs for the networks reference pressure u^{p_0}, and the pressure difference for the producer $u_s^{\Delta p}$. For all three control inputs, we impose simple box constraints

$$u_s^{e,min} \leq u_s^e \leq u_s^{e,max}, \tag{2.90a}$$
$$u_s^{\Delta p,min} \leq u_s^{\Delta p} \leq u_s^{\Delta p,max}, \tag{2.90b}$$
$$u_s^{p_0,min} \leq u_s^{p_0} \leq u_s^{p_0,max}, \tag{2.90c}$$

as well as a mixed supply power box constraint

$$0 < \Delta Q_s^{min} \leq Q_{s:in} + Q_{s:out} \leq \Delta Q_s^{max}, \tag{2.91}$$

which involve both, state and control variables. Here we emphasize, that we only directly control the energy input, and pressure levels, whereas flow velocities (and volume/mass fluxes) are completely determined by the network's internal dynamics. Therefore, we often can not easily find a set of control inputs, which satisfy (2.91), as a validation of feasibility usually involves a full numerical simulation.
To be consistent with the notation introduced in SECTION 2.2, we define the symbols

$$e_{s:in} = e_{i(s)}, \tag{2.92}$$
$$e_{s:out} = u_s^e, \tag{2.93}$$

for the inlet and outlet energies.

2.6 Summary: The complete model

For each pipe $a \in \mathcal{A}_P$, we solve the energy transport and pressure difference equations

$$\partial_t e_a + \partial_x \left(v_a e_a\right) = -r_a\left(e_a\right), \tag{2.94a}$$

$$p_{o(a)} - p_{i(a)} = -\left(g\frac{\Delta h_a}{L_a} + \frac{\lambda_a}{2d_a} v_a \left|v_a\right|\right) \int_{\Omega_a} \rho\left(e_a\right)\, dx, \tag{2.94b}$$

with fluxes, initial and boundary conditions

$$e_{a:in} = e_{i(a)}, \tag{2.95a}$$

$$e_a(t_0, \cdot) = e_a^{init}, \tag{2.95b}$$

$$p_{a:in} = p_{i(a)} \tag{2.95c}$$

$$p_{a:out} = p_{o(a)}, \tag{2.95d}$$

$$q_{a:in} = -A_a v_a, \tag{2.96a}$$

$$q_{a:out} = A_a v_a, \tag{2.96b}$$

$$Q_{a:in} = q_{a:in} e_{a:in}, \tag{2.96c}$$

$$Q_{a:out} = q_{a:out} e_{a:out}, \tag{2.96d}$$

If the initial state e_a^{init} is not known, one can add the stationary advection problem

$$v_a(t_0)\partial_x e_a^{init,} = -r_a\left(e_a^{init}\right), \tag{2.97a}$$

$$e_a^{init}(0) = e_{i(a)}\left(t_0\right), \tag{2.97b}$$

to the equation system.

For each consumer $c \in \mathcal{A}_C$, we couple mass an energy fluxes according to

$$\rho\big(\phi_c\big(e_{i(c)}\big)\big) q_{c:in} + \rho\big(e_c^{ret}\big) q_{c:out} = 0 \tag{2.98a}$$

$$Q_{c:in} + q_{c:in}\phi_c\big(e_{i(c)}\big) = 0 \tag{2.98b}$$

$$Q_{c:out} + q_{c:in} e_c^{ret} = 0 \tag{2.98c}$$

$$Q_{c:in} + Q_{c:out} + \Delta Q_c^{pred} = 0 \tag{2.98d}$$

$$e_c^{min} \le e_{i(c)} \le e_c^{max}, \tag{2.99a}$$

$$p_c^{min} \le p_{i(c)} \le p_c^{max}, \tag{2.99b}$$

$$\Delta p_c^{min} \le p_{o(c)} - p_{i(c)} \tag{2.99c}$$

where we require additional state constraints to be satisfied in order to guarantee problem-free functionality of the heat exchangers.

For the producer s, the control inputs are coupled with the rest of the network by a linear system of equations

$$Q_{s:in} = q_{s:in} e_{i(s)} \tag{2.100a}$$

$$Q_{s:out} = q_{s:out} u^e \tag{2.100b}$$

$$p_{i(s)} = u_s^{p_0} \tag{2.100c}$$

$$p_{o(s)} - p_{i(s)} = u_s^{\Delta p} \tag{2.100d}$$

$$u_s^{e,min} \le u_s^e \le u_s^{e,max} \tag{2.101a}$$

$$u_s^{p,min} \le u_s^{p_0} \le u_s^{p,max} \tag{2.101b}$$

$$u_s^{\Delta p,min} \le u_s^{\Delta p} \le u_s^{\Delta p,max} \tag{2.101c}$$

$$Q_{s:in} + Q_{s:out} \le \Delta Q_s^{max}. \tag{2.101d}$$

The box constraints for control variables, and the mixed, bilinear constraint are supposed to ensure a realizability of the reference curves by the district heating plants control systems.

For each node $n \in \mathcal{N}$ we require, that the conservation laws

$$\sum_{a \in I_n} \rho\left(e_{a:n}\right) q_{a:n} = 0, \tag{2.102}$$

$$\sum_{a \in I_n} Q_{a:n} = 0, \tag{2.103}$$

for mass and energy fluxes are fulfilled.

Chapter 3

Analysis and H^1 formulation

Now, that we have set up a system of equations describing the district heating network's dynamical behaviour, we are going to analyse its solvability, and derive a rigorous mathematical model which is suitable for optimization problems.
Our first goal is to examine, under which conditions the system (2.94a) - (2.103) has a solution, and whether it is unique. In particular, we study existence and uniqueness results in different function spaces such that we can choose the one which we consider the most practical within the context of optimal control problems.
We start with the scalar advection equation

$$\partial_t e + v\partial_x(e) + r(e) = 0, \tag{3.1a}$$
$$e(t_0, \cdot) = e^{init}, \tag{3.1b}$$
$$e(\cdot, 0) = e^{in}, \tag{3.1c}$$

whose classical solution (see e.g. [LeVeque, 2008], [Evans, 2010]) is well known and has an explicit representation formula using characteristics, if v is positive, and sufficiently regular.
We expect the same to hold true, if we add a simple consumer model

$$v\left(e(\cdot, L) - e^{ret}\right) = g \tag{3.2}$$

to the system (3.1), which can be interpreted as a *non-local boundary condition* defining the advection velocity v. This becomes more obvious, if we eliminate the consumer equation, and obtain the non-local conservation law

$$\partial_t e + \partial_x e \int_\Omega k(e; t, x)\, dx = 0 \tag{3.3a}$$
$$k(e; t, x) = \frac{g(t)}{\delta(x - L)\left(e(t, x) - e^{ret}\right)} \tag{3.3b}$$
$$e(t_0, \cdot) = e^{init}, \tag{3.3c}$$
$$e(\cdot, 0) = e^{in}, \tag{3.3d}$$

with singular kernel. Here we can already recognize, that the *trace evaluation* $e(\cdot, L)$ needs to be well-defined. We also notice, that we take the non-local point of view to gain intuition for the systems dynamical behaviour, and we prefer the coupled system (3.1)-(3.2) for our analytic examination. In the upcoming SECTION *3.1*, we establish a suitable notion of a solution to the equation, which is then generalized to *simple networks* (in terms of DEFINITION *2.6*), in SECTION *3.2*.

Finally, we define appropriate Banach spaces $\mathcal{U}$, $\mathcal{Y}$, $\mathcal{Z}$, and the abstract residual and solution operators

$$\mathcal{G} : \mathcal{U} \times \mathcal{Y} \longrightarrow \mathcal{Z}^\star, \qquad \mathcal{S} : \mathcal{U} \longrightarrow \mathcal{Y}, \tag{3.4}$$

such that $\mathcal{G}(\mathbf{u}, \mathbf{y}) = 0$ holds, if and only if $\mathbf{y} = \mathcal{S}\mathbf{u}$. This formulation should be equivalent to solutions of (2.94) - (2.103) in the sense of the theory presented in SECTION 3.1 and SECTION 3.2, if appropriate boundary conditions are given.
For applications in both abstract and numerical optimization, we would like the *dual pairings*

$$\langle \mathcal{G}(\mathbf{u}, \mathbf{y}), \mathbf{z} \rangle_{\mathcal{Z}^\star, \mathcal{Z}}, \qquad \langle \mathcal{G}_{\mathbf{u}}(\mathbf{u}, \mathbf{y}), \mathbf{z} \rangle_{\mathcal{Z}^\star, \mathcal{Z}}, \qquad \langle \mathcal{G}_{\mathbf{y}}(\mathbf{u}, \mathbf{y}), \mathbf{z} \rangle_{\mathcal{Z}^\star, \mathcal{Z}}, \tag{3.5}$$

to be well defined, and take a form which is convenient for the derivation of the *adjoint state equations* (i.e. the adjoint of the linearized residual operator), and their numerical solution. Here, $\mathcal{Z}^\star$ denotes the *topological dual space* of $\mathcal{Z}$. In particular, this requires $\mathcal{G}$ to be bounded, continuous, and (at least one time) continuously *Fréchet differentiable* (see SECTION 3.3). A structured overview over these different approaches and results is shown FIGURE 3.1.

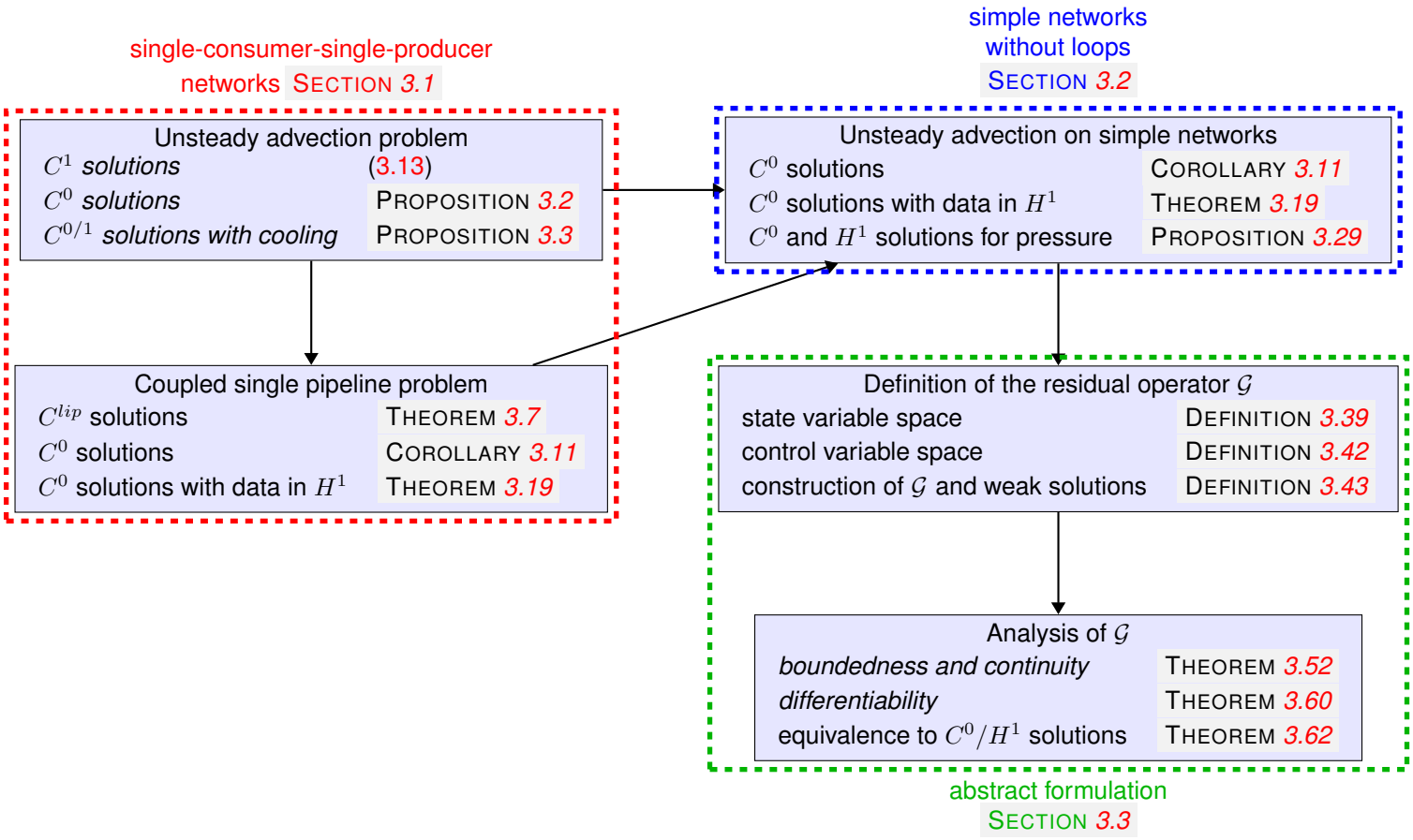

Figure 3.1: Structure of this chapter: From the scalar advection problem to an abstract formulation for simple networks

In the following, we always assume $I_t = (t_0, t_f)$ to be the time domain of our model, and $\Omega = (0, L)$ the spatial domain of a pipeline ($\Omega_a = (0, L_a)$, if a specific pipe $a \in \mathcal{A}_P$ is addressed). We denote by $C^0(\bar{M})$, and $C^k(M)$ the classical function spaces of continuous, and k times continuously differentiable, real-valued functions, where $M \subset \mathbb{R}^d$ is open and bounded (see, e.g. [Rudin, 1986]). Given any Banach space X, we denote its norm by $\|\cdot\|_X$. If X is a Hilbert space, we denote its scalar product by $(\cdot,\cdot)_X$. Further, $L^p(M)$, and $H^k(M) = W^{k,2}(M)$ denote the usual *Lebesgue* and *Sobolev Hilbert spaces* (see e.g. [Evans, 2010], [Brezis, 2011]).

3.1 Single-Consumer-Single-Producer Networks

The single pipeline network (depicted in FIGURE 3.2) consists of a consumer, a producer and a pipeline. The return network is contracted to a single node, making this the simplest possible network within the framework of CHAPTER 2.

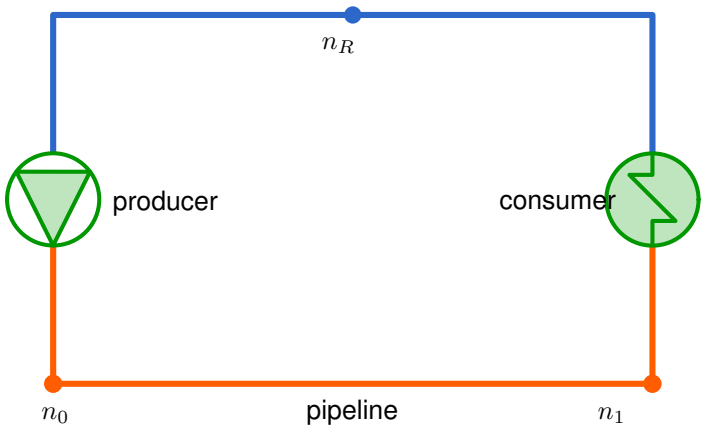

Figure 3.2: Smallest possible simple district heating network following definition DEFINITION 2.6, consisting of a single pipeline, producer, and consumer. The return flow network (blue) consists of only one node n_R.

With the assumption, that ρ is constant, we can eliminate all flux and node variables, and the governing equations can be formulated as a system

$$\partial_t e + v\partial_x e = -r(e) \qquad \text{in } I_t \times \Omega, \tag{3.6a}$$
$$e = e^{in} \qquad \text{in } \bar{I}_t \times \{0\}, \tag{3.6b}$$
$$e = e^{init} \qquad \text{in } \{t_0\} \times \bar{\Omega}, \tag{3.6c}$$
$$v\left(e - e^{ret}\right) = g \qquad \text{in } \bar{I}_t \times \{L\}, \tag{3.6d}$$

in the space-time domain $I_t \times \Omega = (t_0, t_f) \times (0, L)$, for which we want to prove existence and uniqueness of a solution (e, v) in an appropriate setting.
Here, the function

$$g(t) = \frac{\Delta Q^{pred}(t)}{\frac{\pi}{4}d^2}. \tag{3.7}$$

denotes the cross section averaged consumer demand.

3.1.1 Characteristics and continuous solutions of the advection equation

Before we study the fully coupled single consumer network, we consider the unsteady advection problem

$$\partial_t e + v\partial_x e + r(e) = 0 \qquad \text{in } (t_0,\infty)\times(0,L), \tag{3.8a}$$
$$e = e^{init} \qquad \text{in } \{t_0\}\times[0,L], \tag{3.8b}$$
$$e = e^{in} \qquad \text{in } [t_0,\infty)\times\{0\}, \tag{3.8c}$$

with initial data $e^{init} \in C^1((0,L))$, and boundary data $e^{in} \in C^1((t_0,\infty))$. Furthermore, we assume that the advection velocity is a continuous function $v \in C^0([t_0,\infty))$, satisfying a lower bound condition $v(t) \geq v^{min} > 0$.
A possible approach to solve this equation is provided by the *method of characteristics* (see [Alinhac, 2009], [LeVeque, 2008], or [Hörmander, 1997] for a broader introduction into this topic)

$$\frac{dt}{ds} = 1, \qquad t(0) = \tau, \tag{3.9a}$$
$$\frac{dx}{ds} = v(s), \qquad x(0) = \xi, \tag{3.9b}$$
$$\frac{de}{ds} = -r(e), \qquad (\tau,\xi) \in \Sigma, \tag{3.9c}$$

where the origin coordinates $(\tau,\xi) \in \{t_0\}\times[0,L]\cup[t_0,\infty]\times\{0\} := \Sigma$ are points on the *hyperbolic boundary* of our space-time domain.
We can directly integrate the first two equations (3.9a)-(3.9b) and obtain closed form solutions

$$t(s) = \tau + s, \tag{3.10a}$$
$$x(s) = \xi + \int_0^s v(\tilde{s})\,d\tilde{s} = \xi + \int_\tau^t v(\tilde{t})\,d\tilde{t}, \tag{3.10b}$$

for the characteristic curves.
We define the set

$$D(I_t) = \left\{(t,x) \in I_t\times\Omega \;\middle|\; \int_{t_0}^t v(s)\,ds - x \in \Omega\right\} \tag{3.11}$$

of points $(t,x) \in I_t\times\Omega$ which are reachable from $\Omega_0 = \{t_0\}\times\Omega \subset \Sigma$ in finite time.
We can see, that if $(t,x) \in D(I_t)$, there always exists a characteristic curve with origin coordinates (t_0,ξ), which passes through the point (t,x). In particular, we can rearrange (3.10b), and obtain

$$\xi(t,x) = x - \int_{t_0}^t v(s)\,ds > 0. \tag{3.12}$$

In the special case $r \equiv 0$, the solution takes the explicit form

$$e(t,x) = e^{init}(\xi(t,x)) = \tilde{e}^{init}\left(x - \int_{t_0}^t v(s)\,dx\right). \tag{3.13}$$

On the other hand, for every point $(t,x) \in D^c(I_t) = I_t\times\Omega\setminus D(I_t)$ in the complement set of $D(I_t)$, such a point cannot exist. The properties of v ensure, that the equation

$$\int_{\tau(t,x)}^t v(s)\,ds - x = 0 \tag{3.14}$$

always has a unique positive solution $t_0 < \tau(t,x) < t_f$.
Putting both parts together, we can conclude that

$$\xi(t,x) = \max\left\{x - \int_{t_0}^{t} v(s)\,ds, 0\right\} \tag{3.15}$$

and

$$\tau(t,x) = \begin{cases} t_0, & \text{if } x \geq \int_{t_0}^{t} v(s)\,ds \\ \text{solution of } \int_{\tau}^{t} v(s)\,ds = x, & \text{else,} \end{cases} \tag{3.16}$$

are the origin coordinates for the unique characteristic curve passing through the point $(t,x) \in \bar{I}_t \times \bar{\Omega}$ in the closed space time domain. In the special case $r \equiv 0$, this yields the general solution of (3.8)

$$\begin{aligned} e(t,x) &= e\left(\tau(t,x), \xi(t,x)\right) \\ &= \begin{cases} e^{init}\left(\xi(t,x)\right) & , \text{ if} x > \int_{t_0}^{t} v(s)\,ds, \\ e^{in}(\tau(t,x)) & , \text{ else,} \end{cases} \end{aligned} \tag{3.17}$$

provided that e^{in}, and e^{init} satisfy the appropriate compatibility conditions

$$\lim_{t \searrow t_0} \frac{d^k e^{in}}{dt^k}(\tau(t,0)) = \lim_{x \searrow 0} \frac{d^k e^{init}}{dx^k}(\xi(t_0,x)) \tag{3.18}$$

up to the desired order $k \geq 1$.
In the case $k = 0$, it immediately follows, that we require

$$e^{init}(0) = e^{inflow}(t_0) \tag{3.19}$$

for $e(t,x)$ provided by (3.17) to be continuous. Implicit differentiation of the equation (3.14) gives us the relation

$$\frac{d\tau(t,x)}{dx} = -v(\tau(t,x)) \tag{3.20}$$

such that we can derive compatibility conditions

$$\frac{de^{init}}{dx}(0) + v(t_0)\frac{de^{in}}{dt}(t_0) = 0, \tag{3.21}$$

for continuously differentiable solutions. We note, that (3.19)-(3.21) are only necessary, if one wishes to solve (3.8) in the classical sense, but the solution formula (3.17) still yields a well defined, continuous function, if only the first condition is imposed. Therefore, it can be thought of as a generalized (or weaker) solution of (3.8).

Remark 3.1: Higher order coupling terms

Theoretically, (3.18) can yield compatibility conditions up to an arbitrary order. In the case of C^2 solutions, the data need to satisfy

$$\begin{aligned} 0 &= v(t_0)^2 \frac{d^2 e^{init}}{dx^2}(0) - \frac{\frac{dv}{dt}(t_0)}{v(t_0)} \frac{de^{in}}{dt}(t_0) + \frac{d^2 e^{in}}{dt^2}(t_0) \\ &= v(t_0)^2 \frac{d^2 e^{init}}{dx^2}(0) + \frac{dv}{dt}(t_0) \frac{de^{init}}{dx}(0) + \frac{d^2 e^{in}}{dt^2}(t_0), \end{aligned} \tag{3.22}$$

which requires v to be at least one time continuously differentiable.

If we summarize all the observations from above, we can formulate the following proposition:

3.2 Proposition (Explicit solution formula for the unsteady advection equation)

Let $v \in C^0(\bar{I}_t)$, such that $v(t) \geq v^{min} > 0$, and $e^{in} \in C^0(\bar{I}_t)$, $e^{init} \in C^0(\bar{\Omega})$, such that (3.19) holds. Then the function e defined by (3.17) is continuous, (i.e. $e \in C^0(\bar{I}_t \times \bar{\Omega})$), and solves (3.8) without reaction term ($r \equiv 0$) in the sense that it is constant along the characteristic curves defined by (3.9a)-(3.9b).
If, in addition, $e^{in} \in C^1(I_t)$, and $e^{init} \in C^1(\Omega)$, such that (3.21) holds, then $e \in C^{(1,1)}(I_t \times \Omega)$ solves the initial boundary value problem (3.8) in the classical sense.

Proof. Both claims follows from the explicit construction of (3.17) given above. □

Before we move on to the general case with an arbitrary, non-zero cooling term, we consider a special version, where we approximate certain thermodynamic quantities by their averages, as described in ASSUMPTION *2.3*. The relation between the temperature T, and energy density e then is an affine linear function

$$T(e) = T_0 + T_1 e \tag{3.23}$$

with positive, real constants T_0, and T_1. For the resulting reaction term

$$r(e) = \underbrace{\frac{4k}{d} T_1}_{r_1} \left(e - e^{wall}\right) \tag{3.24}$$

we can explicitly compute the solution

$$e(t,x) = e^{wall} + \left(e_0(t,x) - e^{wall}\right) \exp\left(-r_1 \left(t - \tau(t,x)\right)\right), \tag{3.25}$$

of (3.8), where $e_0(t,x)$ refers to the unique solution (3.17) of the advection problem without cooling.
For the general case, it is sufficient to assume that r is strictly increasing on a compact interval $[e^{min}, e^{max}]$, with a single zero $r(e^{wall}) = 0$, to justify

$$r(e) \leq r_1 \left(e - e^{wall}\right) \text{ for } e \in [e^{wall}, e^{max}]. \tag{3.26}$$

We use this estimate, to prove a generalized version of PROPOSITION *3.2*:

3.3 Proposition (Solution of the unsteady advection problem with nonlinear reaction term)

Let v, e^{in}, and e^{init} fulfil all requirements of PROPOSITION 3.2*, and*

$$0 < e^{wall} < e^{min} \leq e^{in}(t), e^{init}(x) \leq e^{max} \tag{3.27}$$

holds for all t, x. Further, let $r \in C^1((0, e^{max})) \cap C^0([0, e^{max}])$ be monotonously increasing, and strictly positive on the sub-interval $(e^{wall}, e^{max}]$, whose growth is bounded by a first order polynomial

$$r(e) \leq r_1 \left(e - e^{wall}\right), \tag{3.28}$$

with a positive constant $r_1 > 0$. Then, the problem (3.8) has a unique solution $e \in C^{(1,1)}(I_t \times \Omega) \cup C^0\left(\bar{I}_t \times \bar{\Omega}\right)$, such that $e^{wall} < e \leq e^{max}$. Furthermore, the e depends continuously on the boundary and initial data.

Proof. We follow the method of characteristics with a modified reaction term

$$\tilde{r}(e) = \begin{cases} 0, & r \leq e^{wall} \\ r(e), & e^{wall} < e < e^{max} \\ r\left(e^{max}\right), & e^{max} \leq e \end{cases} \tag{3.29}$$

which is Lipschitz continuous. Then the solution $\tilde{e}(t, x)$ of (3.8) (with modified r) at each point (t, x) is given by the solution of the ordinary differential equation

$$\frac{d\tilde{e}}{ds} + \tilde{r}(e) = 0, \qquad s \in (0, t - \tau(t, x)), \tag{3.30}$$

$$\tilde{e}(0) = \tilde{e}_0, \tag{3.31}$$

with initial value $\tilde{e}_0 = e(t, x)$ provided by the solution formula (3.17) of the problem without reaction term. We now apply the Picard-Lindelöf theorem, which yields the existence and uniqueness of a solution $\tilde{e}$. Because, by assumption, $e^{wall} < \tilde{e}_0 \leq e^{max}$, and $-r$ is strictly negative and decreasing, the solution is strictly decreasing along each characteristic, but cannot attain the value e^{wall} in finite time due to the polynomial bound (3.28): Solving the equation with $R(e) = r_1 \left(e - e^{wall}\right)$ as the reaction term yields a sub-solution of the original problem, and we obtain an estimate

$$\tilde{e}(t, x) \geq e^{wall} + \left(e_0(t, x) - e^{wall}\right) \exp\left(-r_1 \left(t - \tau(t, x)\right)\right) > e^{wall}, \tag{3.32}$$

which proves that e^{wall} always is a strict lower bound. Therefore, the solution satisfies $\tilde{r}(\tilde{e}) = r(\tilde{e})$, and also solves the unmodified problem (3.8), and $e = \tilde{e}$ is the unique solution, which continuously depends on $e_0(t, x)$. Due to PROPOSITION 3.2 we also know, that $e_0(t, x)$ (as defined by (3.17)) is continuous, and continuously depends on e^{in}, and e^{init}, which completes the proof. □

Remark 3.4: Lipschitz continuity

For every point (t, x), the solution fulfils the (scalar) integral equation

$$\int_0^{t-\tau(t,x)} ds = -\int_{e_0(t,x)}^{e(t,x)} \frac{d\lambda}{r(\lambda)}, \tag{3.33}$$

such that we have a pointwise estimate

$$0 < \frac{de(t,x)}{de_0(t,x)} = \frac{r(e(t,x))}{r(e_0(t,x))} \leq \frac{r(e^{max})}{r(e^{min})} := L_S < \infty \tag{3.34}$$

for the sensitivity of $e(t,x)$ w.r.t. $e_0(t,x)$ along each characteristic.
If we implicitly define the solution operator $S : e_0 \mapsto e$, we can estimate the influence of a perturbation $\tilde{e}_0$ of the initial data by

$$\|S(e_0) - S(\tilde{e}_0)\|_\infty \leq L_S \|e_0 - \tilde{e}_0\|_\infty . \tag{3.35}$$

A more general result, which proves the Lipschitz continuity of e w.r.t. e^{in}, e^{init}, and v, is shown in the upcoming section.

3.1.2 Lipschitz solutions of the coupled problem

With an explicit solution formula at hand, we can now approach solving the coupled problem, which adds the non-local boundary condition

$$v(t)\left(e(t,L) - e^{ret}\right) = g(t) \tag{3.36}$$

to the system. According to (3.17), the energy density at the outflow boundary $e^L(v) = e(\cdot, L)$ is uniquely determined by e^{in}, e^{init}, and v, such that we can interpret

$$v(t) = \frac{g(t)}{e^L(v) - e^{ret}} \tag{3.37}$$

as a fixed point equation w.r.t. v. In order to prove existence and uniqueness of a solution, we make use of the following theorem:

3.5 Theorem (Banach Fixed Point Theorem)

Let V be a closed subset of a Banach space X, and $f : V \to V$ a contraction. Then the equation

$$f(x) = x \tag{3.38}$$

has a unique solution in V.

Proof. See e.g. [Evans, 2010]. □

So far, we have not made any assumptions about the properties of initial and boundary data. The fixed point form (3.37) of the consumer equation suggests, that we might run into a problem, if $e(t,L) = e^{ret}$ at some time point, or if the normalized consumption g attains non-positive values. Therefore, we have to make a few assumption, before we proceed with our existence theorem.

Assumption 3.6: Regularity assumptions for Lipschitz solutions

Given initial and boundary data e^{init}, e^{in}, and g , we assume the following:

SP.1 $e^{init} \in C^0(\bar{I}_t)$ with $e^{min} \leq e^{init} \leq e^{max}$

SP.2 $e^{in} \in C^0(\bar{I}_t)$ with $e^{min} \leq e^{in} \leq e^{max}$. Further $e^{in}(t_0) = e^{init}(0)$.

SP.3 $e^{ret} < e^{in,min} \leq e^{min} \leq e^{max} \leq e^{in,max}$

SP.4 $g \in C^0(\bar{I}_t)$ with $0 < g^{min} \leq g \leq g^{max}$

3.7 Theorem (Existence And Uniqueness for a Single Pipeline)

Let e^{init}, e^{in}, and g be data for the coupled advection problem

$$\partial_t e + v\partial_x e = 0, \tag{3.39a}$$
$$e(\cdot, 0) = e^{in}, \tag{3.39b}$$
$$e(t_0, \cdot) = e^{init}, \tag{3.39c}$$
$$v\left(e(\cdot, L) - e^{ret}\right) = g, \tag{3.39d}$$

fulfilling all assumptions in ASSUMPTION 3.6 *. Further assume, that $e^{in} \in C^{lip}(\bar{I}_t)$, and $e^{init} \in C^{lip}(\bar{\Omega})$. Then the there exists a unique solution $(v, e) \in C^0(\bar{I}_t) \times C^{lip}(\bar{I}_t \times \bar{\Omega})$ in the sense of* PROPOSITION 3.3 *(i.e. in the terms of characteristics). If e^{in}, and e^{init} are even continuously differentiable, and satisfy the compatibility condition*

$$\partial_t e^{in}(t_0) + v(t_0)\partial_x e^{init}(0) = 0, \tag{3.40}$$

then $e \in C^{(1,1)}(I_t \times \Omega)$.

Proof. **Step 1: Local Solutions by the Banach Fixed Point Theorem**

By the reformulation of the consumer equation (3.37), we can immediately derive upper and lower bounds

$$v^{min} = \frac{g^{min}}{e^{max} - e^{ret}} \leq v \leq \frac{g^{max}}{e^{min} - e^{ret}} = v^{max} \tag{3.41}$$

of the advection velocity v, and define the set

$$V = \left\{ v \in C^0(I_t) \,\middle|\, v^{min} \leq v \leq v^{max} \right\} \tag{3.42}$$

which is a bounded, and closed subset of $C^0(I_t)$. Within this set, the simplified solution formula (3.13) is well-defined, and the equation (3.37) can be re-written as

$$v(t) = \frac{g(t)}{e^{init}(L - \int_{t_0}^{t} v(s)ds) - e^{ret}} =: f(v) \tag{3.43}$$

with $t \in [t_0, t_0 + \frac{L}{v_{max}})$. The right hand side f is a mapping from V to itself, which is Lipschitz

continuous due to the estimate

$$\begin{aligned}\|f(t,v_1)-f(t,v_2)\|_\infty &= \left\| \frac{g(t)}{e^{init}\left(L-\int_{t_0}^t v_1(s)ds\right)-e^{ret}} - \frac{g(t)}{e^{init}\left(L-\int_{t_0}^t v_2(s)ds\right)-e^{ret}} \right\|_\infty \\ &\leq \frac{\left\| g(t)\left(e^{init}\left(L-\int_{t_0}^t v_1(s)ds\right)-e^{init}\left(L-\int_{t_0}^t v_2(s)ds\right)\right)\right\|_\infty}{\left(e^{min}-e^{ret}\right)^2} \\ &\leq \frac{\|g\|_\infty}{\left(e^{min}-e^{ret}\right)^2}\cdot C_{Lip,e}\cdot \left\| \int_{t_0}^t v_1(s)-v_2(s)\,ds \right\|_\infty \\ &\leq \frac{\|g\|_\infty}{\left(e^{min}-e^{ret}\right)^2}\cdot C_{Lip,e}\cdot |t-t_0|\cdot \|v_1-v_2\|_\infty .\end{aligned} \tag{3.44}$$

As a consequence, there exists $t^\star \in (t_0, t_0+\frac{L}{v^{max}})$, such that f is a contraction. Therefore, all prerequisites from THEOREM *3.5* are met, such that a unique solution $v^\star \in V$ exists within $[t_0, t^\star]$.

Step 2: Lipschitz-Continuity of all intermediate solutions

For this step, lets assume that $(e,\, v)$ is the unique solution to (3.39) on a subinterval $t_0 \leq \underline{s} < \bar{s} \leq t_1$. Assuming Lipschitz continuity of the initial data at $\underline{s}$, the estimate

$$\begin{aligned}\|e(s_2,x)-e(s_1,x)\|_\infty &\leq C_{Lip,e}\left\| x-\int_{\underline{s}}^{s_1} v(t)\,dt - x + \int_{\underline{s}}^{s_2} v(t)\,dt\right\|_\infty \\ &= C_{Lip,e}\left\| \int_{s_1}^{s_2} v(t)\,dt\right\|_\infty \\ &\leq v^{max}\,\|s_2-s_1\|_\infty\end{aligned} \tag{3.45}$$

holds for all $s_1 \neq s_2 \in [\underline{s}, \bar{s}]$, $x \in (0, L]$, such that $\int_{\underline{s}}^{s_i} v\,dt \leq x$. For all positions x where

$$\int_{\underline{s}}^{\bar{s}} v(t)\,dt > x \tag{3.46}$$

we define the time point $s^\star(x)$

$$\int_{\underline{s}}^{s^\star(x)} v(t)\,dt = x \tag{3.47}$$

where one transitions from initial data to boundary data. Given $s_2 > s_1 \geq s^\star(x)$, we can compute the initial time points τ_i of the characteristics passing through the point (s_i, x) by solving

$$\int_{\tau_i}^{s_i} v(t)\,dt = x. \tag{3.48}$$

This yields the second part

$$\begin{aligned}\|e(s_2,x)-e(s_1,x)\|_\infty &= \left\|e^{in}(\tau_2)-e^{in}(\tau_1)\right\|_\infty \\ &\leq C_{Lip,u}\,\|\tau_2-\tau_1\|_\infty \\ &\leq C_{Lip,u}\,\frac{v^{max}}{v^{min}}\,\|s_2-s_1\|_\infty\end{aligned} \tag{3.49}$$

of the desired estimate, such that e is Lipschitz in time. In order to show Lipschitz continuity of e in space let $x_1 < x_2 \in [0, L]$ and $s \geq s_0$. We directly obtain the estimate

$$\|e(s, x_2) - e(s, x_1)\|_\infty \leq C_{Lip,e} \|x_2 - x_1\|_\infty \tag{3.50}$$

in the explicit case (i.e. $\int_{s_0}^{s} v \, dt \leq x_i$), and

$$\begin{aligned} \|e(s, x_2) - e(s, x_1)\|_\infty &\leq C_{Lip,u} \left\| \frac{\partial \tau(t, x)}{\partial x} \right\|_{\infty,x} \|x_2 - x_1\|_\infty \\ &= C_{Lip,u} \frac{1}{v^{min}} \|x_2 - x_1\|_\infty \end{aligned} \tag{3.51}$$

otherwise.

Step 3: Continuation to the whole time interval

Due to the considerations in **Step 1**, we can construct a local, unique solution to the coupled transport problem within any time interval $[t^{(n)}, t^{\star(n)}] \subset [t_0, t_1]$, where $t^{\star(n)}$ is chosen as the maximal element of the set defined by

$$\begin{aligned} \left(t^\star - t^{(n)}\right) \frac{\|g\|_\infty}{\left(e^{min} - e^{ret}\right)^2} \cdot C_{Lip,e} < 1, \\ t^{(n)} \leq t^\star \leq t^{(n)} + \frac{L}{v^{max}}. \end{aligned} \tag{3.52}$$

We observe that the difference $t^{\star(n)} - t^{(n)}$ is a constant independent of n, and define $\Delta t := t^{\star(n)} - t^{(n)}$. This induces a unique partition

$$t^{(n)} = t_0 + n\Delta t, \qquad N_t := \left\lceil \frac{t_1 - t_0}{\Delta t} \right\rceil, \qquad t^{(N_t)} = \min\left(t_1, t_0 + N_t \Delta t\right). \tag{3.53}$$

of the whole time interval. The considerations in **Step 2** ensure that all intermediate solutions are Lipschitz, and therefore satisfy the prerequisites of **Step 1**. By induction, this leads to a unique solution (e, v) of the coupled problem (3.39), with e being Lipschitz, and v being continuous.

Step 4: Classical Solutions

Together with the compatibility condition in ASSUMPTION *3.6*, the differentiability follows immediately from the explicit construction of (3.17). □

Here we notice, that similar techniques, which stem from combining the method of characteristics with Banach's fixed point theorem are commonly used in the context of nonlocal transport equations. For a existence result for conservation laws with nonlocal velocities in a broader context we refer the reader to [Friedrich et al., 2022] .

The preceding theorem ensures the existence of a continuous, bounded, and positive advection velocity under certain conditions. If the consumption model g admits more regularity, we can prove the same for v:

3.8 Corollary (Improved Regularity Results for v)

Let e^{init}, e^{in}, and g satisfy all conditions in ASSUMPTION 3.6*. Further, assume $g \in C^{lip}(I_t)$ as well. Then v is Lipschitz continuous with*

$$C_{Lip,v} = \frac{C_{Lip,e} \cdot C_{Lip,g}}{(e^{min} - e^{ret})^2}. \tag{3.54}$$

If g is even continuously differentiable with bounded derivative, then the same folds for v, and one has

$$\partial_t v = \frac{\partial_t g \cdot e(\cdot, L) - g \cdot \partial_t e(\cdot, L)}{(e(\cdot, L) - e^{ret})^2}. \tag{3.55}$$

Proof. In the Lipschitz case, the statement follows immediately from the fixed point formulation (3.37) of the consumer equation, and the norm estimates in the proof of THEOREM 3.7. If g is continuously differentiable, we apply the quotient derivative rule to (3.37), and obtain the second statement. □

3.1.3 Generalization to continuous solutions

The proof of THEOREM 3.7 relies on the rather strict assumption, that initial and boundary data are at least Lipschitz continuous. For applications in optimal control, we would like to generalize this result to data in $H^1(I_t)$, whose continuous representative only satisfies a weaker Hölder condition. In order to do so, we make use of the following approximation theorem:

3.9 Theorem (Stone-Weierstraß)

Let $[a, b]$ be a real interval, and denote by $C^0([a, b])$ the space of continuous, real-valued functions on $[a, b]$. Assume, that V is a sub-algebra of $C^0([a, b])$, which contains at least one non-zero function. Then V is dense in $C^0([a, b])$ (w.r.to the C^0 norm) if and only if it separates points, i.e.

$$\forall x, y \in [a, b] : x \neq y : \exists f \in V : f(x) \neq f(y). \tag{3.56}$$

Proof. See e.g. [Stone, 1948]. □

3.10 Lemma (Uniform approximation by Lipschitz functions)

Let $f \in C^0([a, b])$ be a continuous function with bounds $f_{min}, f_{max} \in \mathbb{R}$ such that

$$f^{min} \leq f(x) \leq f^{max} \forall x \in [a, b]. \tag{3.57}$$

Then there exists a series $(f_k)_k \subset C^{lip}([a, b])$ satisfying

$$f^{min} \leq f_k(x) \leq f^{max} \forall x \in [a, b] \forall k \in \mathbb{N} \tag{3.58}$$

which uniformly converges to f.

Proof. The space $C^{lip}([a,b])$ is closed under addition and multiplication, since we have

$$\|f+g\|_{C^{lip}} \leq \max\left\{\|f\|_{C^{lip}}, \|g\|_{C^{lip}}\right\} \tag{3.59}$$

and

$$\|f\cdot g\|_{C^{lip}} \leq \|f\|_{C^{lip}} \cdot \|g\|_{C^{lip}}. \tag{3.60}$$

Furthermore, it contains all constant functions, as well as piecewise linear functions, such that the prerequisites of theorem THEOREM 3.9 are fulfilled.
Now denote by $(f_k)_k \subset C^{lip}([a,b],\mathbb{R})$ a sequence of approximating functions satisfying

$$\lim_{k\to\infty} \|f-f_k\|_{C^0} = 0. \tag{3.61}$$

In order to apply the point wise projection onto $[f^{min}, f^{max}]$, notice that

$$\min\{f_1,f_2\} = \frac{f_1+f_2-|f_1-f_2|}{2}, \tag{3.62a}$$

$$\max\{f_1,f_2\} = \frac{f_1+f_2+|f_1-f_2|}{2}, \tag{3.62b}$$

such that $C^{lip}([a,b])$ is closed under these operations. As a consequence, the function

$$\tilde{f}_k = \min\left(f^{max}, \max\left(f_k, f^{min}\right)\right) \tag{3.63}$$

is Lipschitz continuous as well. Since the original function f maps onto $[f^{min}, f^{max}]$ as well, we have the estimate

$$\left\|f-\tilde{f}_k\right\|_{C^0} \leq \|f-f_k\|_{C^0}, \tag{3.64}$$

which completes the proof. □

3.11 Corollary (Existence and uniqueness in C^0)

Let $g \in C^0(\bar{I}_t,\mathbb{R})$, $e^{in} \in C^0(\bar{I}_t\mathbb{R})$, and $e^{init} \in C^0(\Omega,\mathbb{R})$, be positive, bounded functions. Further, assume that a C^0 compatibility conditions

$$e^{in}(t_0) = e^{init}(0), \tag{3.65}$$

and all properties in ASSUMPTION 3.6 *are fulfilled. Then (3.39) has a unique solution (v,e) in $C^0(\bar{I}_t) \times C^0(\bar{I}_t\times\bar{\Omega})$ in the sense of* PROPOSITION 3.3.

Proof. The proof is almost identical to that of THEOREM 3.7. In order to apply Banach's fixed point theorem, we successively approximate e^{init} by a series e_k of Lipschitz functions. This results in a series of fixed point problems

$$v_k(t) = \frac{g(t)}{e_k(L-\int_{t_0}^t v_k(s)ds) - e^{ret}} =: f_k(v_k) \tag{3.66}$$

which each have a unique solution v_k. By the estimate

$$\|v_{k+1}-v_k\|_{C^0} \leq \frac{\|g\|_\infty}{\left(e^{min}-e^{ret}\right)^2}\|e_{k+1}-e_k\|_\infty \tag{3.67}$$

we ensure, that the series v_k indeed converges to a unique function v in C^0. □

As already mentioned in SECTION 2.4, its relatively hard to determine sharp bounds for e^{in}, such that $e(\cdot, L) > e^{ret}$ is guaranteed to hold. As a consequence, we introduced a relaxed consumer model in SECTION 2.4.2, which modifies $e(\cdot, L)$ through a correction function ϕ. Using this modification, we can prove the following:

3.12 Corollary (Continuous solutions with cooling)

Assume, that the reaction term

$$r(e) = \frac{4k}{d}\left(T(e) - T_{wall}\right) \tag{3.68}$$

is strictly monotonously increasing, and bijective with one single root $r(e_{wall}) = 0$, and consider a correction function ϕ, which is at least Lipschitz continuous, and bounded from below such that $\phi(e) \geq e^{crit} > e^{ret}$. Further, consider a modified version of (3.39), where the consumer constraint (3.36) is replaced with

$$v\left(\phi\left(e(\cdot, L)\right) - e^{ret}\right) = g. \tag{3.69}$$

Then the modified system has a unique, continuous solution (e, v), which is bounded.

Proof. Due to the properties of the reaction term r, we see that

$$\inf_{(t,x)} |e(t,x)| \geq e^{wall}. \tag{3.70}$$

Further, the relaxation function ϕ is (at least) Lipschitz, such that the modified fixed point problem

$$\tilde{f}(v) = \frac{g(t)}{\phi\left(e^{init}(L - \int_{t_0}^{t} v(s)ds)\right) - e^{ret}} \tag{3.71}$$

is Lipschitz as well. Therefore, we can proceed as in the proof of COROLLARY 3.11, and conclude the existence and uniqueness of a fixed point $\tilde{f}\left(v^\star\right) = v^\star$. Further, the solution is bounded, where the lower bound

$$e^{wall} \leq \tilde{e}^{min} \leq e^{min} \tag{3.72}$$

of e, and the upper bound

$$\frac{g^{max}}{\phi\left(\tilde{e}^{min}\right) - e^{ret}} =: \tilde{v}^{max} \geq v^{max} \tag{3.73}$$

of v have to be modified, while all other bounds remain exactly the same. □

Remark 3.13: Estimates for affine reaction terms

If the chosen material law leads to an affine relation

$$T(e) = T_0 + T_1 e, \tag{3.74}$$

the reaction term is affine as well. In fact, the condition $r(e^{wall}) = 0$ implies, that r must be of the form

$$r(e) = r_1\left(e - e^{wall}\right) \tag{3.75}$$

for a positive, real constant r_1. By using the estimate $t-\tau(t,x) \leq \frac{L}{v^{min}}$, we can derive a lower bound

$$\begin{aligned} e(t,L) &= e^{wall} + \left(e_0(t) - e^{wall}\right) \exp\left\{-r_1\left(t-\tau(t,L)\right)\right\} \\ &\geq e^{wall} + \left(e_0(t) - e^{wall}\right) \exp\left\{-r_1 \frac{L}{v^{min}}\right\} \end{aligned} \tag{3.76}$$

for the outflow energy. Unfortunately, this estimate is not very sharp, such that it is very unlikely, that it yields a practically usable lower bound, if multiple pipelines are involved. Given a path $(a_0, \ldots, a_N)$ of pipelines, such that $e_{a_k}(t,0) = e_{a_{k-1}}(t, L_{a_{k-1}})$, the above estimate generalizes to

$$\begin{aligned} e_{a_N}(t, L_{a_N}) &= e^{wall} + \left(e_{a_0}(t,0) - e^{wall}\right) \cdot \exp\left\{-\sum_{k=0}^{N} r_{a_k,1}\left(t - \tau_{a_k}(t, L_{a_k})\right)\right\} \\ &\geq e^{wall} + \left(e_{a_0}(t,0) - e^{wall}\right) \cdot \exp\left(-\sum_{k=0}^{N} r_{a_k,1} \frac{L_{a_k}}{v_{a_k}^{min}}\right), \end{aligned} \tag{3.77}$$

and therefore the approximation error propagates in a multiplicative fashion.

So far, we have established different results regarding existence, uniqueness and regularity of solutions of the single pipeline problem with reaction term. Most notable, we could prove the existence of solutions for continuous data. In the following section, we are going to re-add a bit of regularity, to develop a solution framework which is suitable for optimization problems.

3.1.4 Continuous solutions with data in H^1

In the previous section we have seen, that our intuitive understanding of solutions for the coupled pipeline consumer system in terms of characteristics remains valid, if we reduce the regularity of data do "*just*" continuous functions.
As motivated in the introduction of this chapter, we want to establish a weak formulation of the model equations, which capture most good properties of the classical solution, but endows them with a nicer geometry. Since all spatial and temporal domains, which are relevant to our problem, are (compact) intervals, the Sobolev spaces $H^1(I_t)$, and $H^1(\Omega)$ are good candidates for slightly more regular initial and boundary data.
For a broader introduction into Sobolev spaces, their properties, and embeddings, we refer to [Evans, 2010], and [Brezis, 2011].
We start out with two simple observations regarding Sobolev functions on real intervals.

3.14 Lemma (Properties of $H^1(M)$)

Let $M \subset \mathbb{R}$ be an open, real interval. Then the following statements hold true:

1. *The embedding $C^\infty(\bar{M}) \hookrightarrow H^1(M)$ is dense.*
2. *The embeddings $H^1(M) \hookrightarrow C^0(\bar{M})$ and $H^1(M) \hookrightarrow L^2(M)$ are compact.*
3. *$H^1(M)$ is closed under pointwise multiplication. In particular, the triplet $(H^1(M), +, \cdot)$ defines a commutative ring, with the constant function $\mathbf{1}(x) \equiv 1$ as the multiplicative unit element.*

Proof. For the statements (1) and (2), we refer to [Wloka, 1987] and [Alt, 2016]. We are going to prove the third statement. The tuple $\left(H^1(M), +\right)$ defines a commutative group, because $H^1(M)$ is a $\mathbb{R}$-vector space. The existence of a 1-element, and the distributive laws follow immediately from the properties of pointwise multiplication. It remains to show, that for all $f, g \in H^1(M)$, the product also satisfies $f \cdot g \in H^1(M)$.
We know that both functions have unique, continuous representatives, such that we can estimate the L^2 norm of their product by

$$\|fg\|_{L^2(M)} \leq \|f\|_\infty \|g\|_\infty \sqrt{|M|}. \tag{3.78}$$

Now, we are going to show that the distributional derivative of $f \cdot g$ can be identified with a function L^2. Let $g_n \in C_c^\infty(M)$ such that $\|g - g_n\|_{H^1(M)} \to 0$ as $n \to \infty$. Using the product rule for a H^1 and C_c^∞ functions, and estimates analogue to (3.78), the weak derivative f' of f satisfies

$$\begin{aligned} (f' \cdot g_n, \phi)_{L^2} &= (f', g_n \cdot \phi)_{L^2} \\ &= -\left(f, (g_n \cdot \phi)'\right)_{L^2} \\ &= -\left(f, g_n' \cdot \phi + g_n \cdot \phi'\right)_{L^2} \end{aligned} \tag{3.79}$$

for all $\phi \in C_c^\infty(M)$, which we rearrange to

$$(fg_n, \phi')_{L^2} = -\left(f'g_n + fg_n', \phi\right)_{L^2}. \tag{3.80}$$

For $g_n \in H^1(M)$, all three expressions

$$\begin{aligned} g_n &\mapsto (g_n, f \cdot \phi')_{L^2} \\ g_n &\mapsto (g_n, f' \cdot \phi)_{L^2} \\ g_n &\mapsto (g_n', f \cdot \phi)_{L^2} \end{aligned} \tag{3.81}$$

define continuous, linear functionals in $H^1(M)^\star$. Since the strong convergence of g_n also implies weak convergence, all limits necessarily exist in $H^1(M)$, and we conclude that $f \cdot g \in H^1(M)$. □

Remark 3.15: Polynomials in H^1

A direct consequence of LEMMA 3.14 is, that formal polynomial expressions

$$P(f) = \sum_{k=0}^{N} a_k f^k \tag{3.82}$$

define mappings from $H^1(M)$ to itself. Furthermore, integrals of the form

$$\mathcal{J}_P(f) = \int_M P(f)(t)\, dt \tag{3.83}$$

are well defined, and Fréchet differentiable (as we are going to show later in SECTION 3.3).

3.16 Lemma (Chain rule for H^1)

Let $D, M \subset \mathbb{R}$ be real intervals, and $f \in H^1(M)$, with $f(x) \in D$ for a.e. $x \in M$. Further, let $F : D \to \mathbb{R}$ be bi-Lipschitz. Then F is differentiable almost everywhere in D, and the composition $F \circ f \in H^1(M)$ satisfies the chain rule

$$\partial_x (F \circ f)(x) = (F\prime \circ f)(x) \cdot \partial_x f(x) \tag{3.84}$$

for almost every $x \in M$. Analogously, if $F : D \to M$ is bi-Lipschitz, then F is differentiable almost everywhere in D, and the composition $f \circ F \in H^1(D)$ satisfies the chain rule

$$\partial_x (f \circ F)(x) = (\partial_x f) \circ F(x) \cdot F'(x) \tag{3.85}$$

for almost every $x \in M$.

Proof. See [Ziemer, 1989], *Theorem 2.2.2* □

Remark 3.17: Quotient rule for H^1

If $g \in H^1(M)$ such that $g \geq g^{min} > 0$, and we define the function

$$F : (g^{min}, \infty) : \mathbb{R}, x \mapsto \frac{1}{x}, \tag{3.86}$$

we see that F is a continuously differentiable (with bounded derivative), and the composition $F \circ g$ has a weak derivative

$$\partial_x \left(F \circ g\right)(x) = -\frac{1}{g(x)^2} \in L^2(M). \tag{3.87}$$

More generally, for any $f \in H^1(M)$, the quotient $\frac{f}{g}$ is well defined, and weakly differentiable with

$$\partial_x \left(\frac{f}{g}\right)(x) = \frac{\partial_x f(x) \cdot g(x) + f(x) \cdot \partial_x g(x)}{g(x)^2} \in L^2(M). \tag{3.88}$$

We now use these results to derive H^1-norm estimates for the partial evaluations $e(t,\cdot)$, and $e(\cdot,x)$ of the (continuous) solution of the advection problem.

3.18 Lemma (Change of coordinates for the advection problem in H^1)

Let $v \in C^0(\bar{I}_t)$ such that $v^{max} \geq v \geq v^{min} > 0$, and define the sets $I_0^{impl} = (t_0, s) \subset I_t$, and

$$\Omega_s^{impl} \coloneqq \left\{ x \in \Omega \,\middle|\, \int_{t_0}^{s} v(t')\,dt' < x \right\} \subset \Omega \tag{3.89}$$

for $s \in I_t$. Then, the mapping

$$\varphi_s : \bar{\Omega}_s^{impl} \to \bar{I}_0^{impl}, x \mapsto \tau(s,x) : \int_{\tau(s,x)}^{s} v(t')\,dt' - x = 0 \tag{3.90}$$

is well defined, and induces a continuous, linear operator

$$\Phi_s : H^1\big(\Omega_s^{impl}\big) \to H^1\Big(I_0^{impl}\Big), u \mapsto u \circ \varphi_s. \tag{3.91}$$

Analogously, we define $\Omega_0^{impl} = (0, x) \subset \Omega$, and

$$I_x^{impl} \coloneqq \left\{ s \in I_t \,\middle|\, \int_{t_0}^{s} v(t')\,dt' < x \right\} \subset I_t \tag{3.92}$$

for $x \in \Omega$. Then, the mappings

$$\vartheta_x : \bar{I}_x^{impl} \to \bar{\Omega}_0^{impl}, t \mapsto \xi(t,x) = x - \int_{t_0}^{t} v(t')\,dt', \tag{3.93}$$

and

$$\zeta_x : \bar{I}_x^{expl} \to \bar{I}_0^{expl}, t \mapsto \tau(t,x) : \int_{\tau(t,x)}^{t} v(t')\,dt' - x = 0 \tag{3.94}$$

are diffeomorphisms, such that the operators

$$\Theta_x : H^1\big(I_x^{impl}\big) \to H^1\Big(\Omega_0^{impl}\Big), u \mapsto u \circ \vartheta_x, \tag{3.95}$$

and

$$\Xi_x : H^1\big(I_x^{expl}\big) \to H^1\Big(I_0^{expl}\Big), u \mapsto u \circ \vartheta_x, \tag{3.96}$$

are linear and continuous, as well.

Proof. A visualisation of the domain subdivisions is given in FIGURE 3.3. Let $s \in I_t$ be arbitrary but fixed. We define the residual equation

$$G(\tau, s, x) \coloneqq \int_{\tau}^{s} v(t')\,dt' - x = 0, \tag{3.97}$$

and obtain

$$\varphi_s'(x) = \frac{1}{v(\varphi_s(x))} \tag{3.98}$$

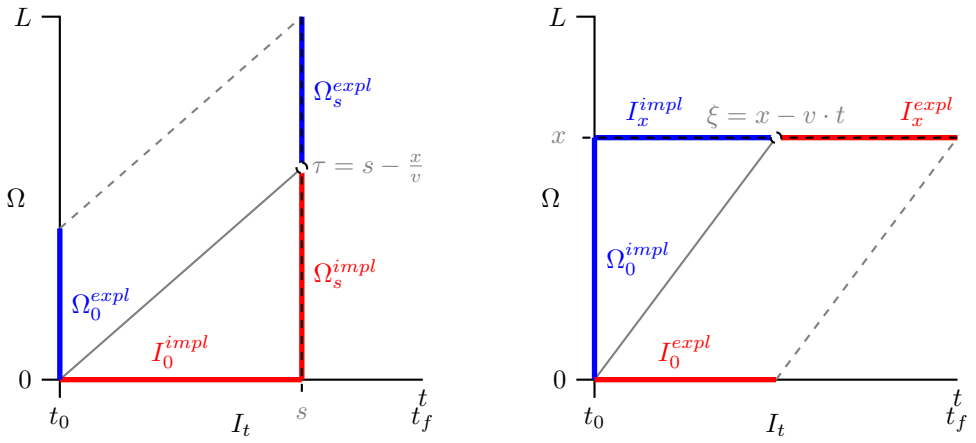

Figure 3.3: Illustration of the domain subdivisions used in LEMMA *3.18* and THEOREM *3.19*

by applying the implicit differentiation theorem, As of LEMMA *3.16*, the composition $u \circ \phi_s$ is an element of $H^1\left(I_0^{impl}\right)$, and

$$\partial_x(\Phi_s u) = (\partial_x u) \circ \varphi(x) \cdot \varphi'(x) \tag{3.99}$$

almost everywhere in Ω_s^{impl}.
This yields the estimate

$$\|\Phi_s u\|_{H^1\left(I_0^{impl}\right)} = \|u \circ \varphi_s\|_{H^1\left(\Omega_s^{impl}\right)} \leq \frac{1}{v^{min}} \|u\|_{H^1\left(I_0^{impl}\right)}, \tag{3.100}$$

for the norm of $\Phi_s u$, such that Φ_s is bounded. We easily see that Φ_s is linear, since $(u_1 + u_2) \circ \varphi_s = u_1 \circ \varphi_s + u_2 \circ \varphi_s$. Therefore, it is also continuous.
Analogously, given $x \in \Omega$ arbitrary but fixed, one shows that

$$\vartheta_x'(t) = -v(t) \tag{3.101}$$

and

$$\zeta_x'(t) = \frac{v(t)}{v(\zeta_x(t))}, \tag{3.102}$$

such that the norm estimates

$$\|\Theta_x u\|_{H^1\left(I_x^{impl}\right)} = \|u \circ \vartheta_x\|_{H^1\left(I_x^{impl}\right)} \leq v^{max} \|u\|_{H^1\left(\Omega_0^{impl}\right)}, \tag{3.103}$$

and

$$\|\Xi_x u\|_{H^1\left(I_x^{expl}\right)} = \|u \circ \vartheta_x\|_{H^1\left(I_x^{expl}\right)} \leq \frac{v^{max}}{v^{min}} \|u\|_{H^1\left(I_0^{expl}\right)}, \tag{3.104}$$

for the linear operators Θ_x and Ξ_x, which hence are continuous. □

We apply this transformation rule to obtain a vastly improved regularity result for e, if the initial and boundary values e^{init} and e^{in} are H^1 functions.

3.19 Theorem (Regularity of C^0 solutions with H^1 data)

Let (v, e) be a continuous solution of the coupled single pipeline problem, as stated in COROLLARY 3.11. *Further, let $e^{in} \in H^1(I_t)$, and $e^{init} \in H^1(\Omega)$. Then $e \in H^{(1,1)}(I_t \times \Omega) \cap C^0\big(\bar{I}_t, H^1(\Omega)\big)$, and the trace operator (spatial point evaluation)*

$$tr_x : \bar{\Omega} \times H^{(1,1)}(I_t \times \Omega) \to H^1(I_t), e \mapsto e(\cdot, x) \tag{3.105}$$

is well defined, and preserves weak differentiability in the sense of Sobolev spaces. In particular, $e^{out} = e(\cdot, L)$ is an element of $H^1(I_t)$.

Proof. First, we want to show that $e \in H^{(1,1)}(I_t \times \Omega)$, i.e. that

$$\|e\|^2_{H^{(1,1)}(I_t \times \Omega)} = \int_{I_t} \int_{\Omega} e(t,x)^2 + \left(\partial_t e(t,x)\right)^2 + \left(\partial_x e(t,x)\right)^2 \, dx \, dt < \infty \tag{3.106}$$

We apply the subdivision given in FIGURE 3.3, which yields

$$\int_{I_t} \int_{\Omega} e(t,x)^2 \, dx \, dt = \int_{I_t} \left(\int_{\Omega_t^{expl}(t)} e(t,x) \, dx + \int_{\Omega_t^{impl}(t)} e(t,x)^2 \, dx \right) dt \tag{3.107}$$

$$= \int_{I_t} \left(\int_{\Omega_0^{expl}(t)} e^{init}(\tilde{x})^2 \, d\tilde{x} + \int_{I_t 0^{impl}(t)} \left(\Phi_s^{-1} e^{in}(s)\right)^2 \, ds \right) dt \tag{3.108}$$

for the first term. Knowing, that the operators Φ_s^{-1} are linear, and diffeomorphisms, we can conclude that the weak partial derivative terms are well defined, and we can analogously apply the subdivision, which yields the desired result.
In order to see that $e \in C^0\big(\bar{I}_t, H^1(\Omega)\big)$, we remind ourselves, that e is continuous by assumption. Therefore, $e \in C^0\big(\bar{I}_t \times \bar{\Omega}\big) \cong C^0\big(\bar{I}_t, C^0(\bar{\Omega})\big)$, where we define the time evaluation $e(t)$ as

$$e(t)(x) = e(t,x) \forall t \in \bar{I}_t, x \in \bar{\Omega}. \tag{3.109}$$

This way, we naturally get the embeddings $e \in C^0\big(\bar{I}_t, L^2(\Omega)\big)$, and $e \in L^2(I_t \times \Omega)$.
We again apply the domain subdivision given in FIGURE 3.3 and LEMMA 3.18.
Now, let $s \in I_t$ be arbitrary but fixed. By LEMMA 3.18, we have the norm estimate

$$\begin{aligned} \|e(s)\|_{H^1(\Omega)} &\leq \|e(s)\|_{H^1\left(\Omega_s^{impl}\right)} + \|e(s)\|_{H^1\left(\Omega_s^{expl}\right)} \\ &\leq \left\|e^{init}\right\|_{H^1\left(\Omega_0^{expl}\right)} + \frac{1}{v^{min}} \left\|e^{in}\right\|_{H^1\left(I_0^{impl}\right)} \\ &\leq \left\|e^{init}\right\|_{H^1(\Omega)} + \frac{1}{v^{min}} \left\|e^{in}\right\|_{H^1(I_t)} \end{aligned} \tag{3.110}$$

such that $e(t) \in H^1(\Omega)$ for every $t \in \bar{I}_t$, and hence $e \in C^0\big(\bar{I}_t, H^1(\Omega)\big)$.
For the last claim, we pick $x \in \bar{\Omega}$ arbitrary, but fixed. Again, LEMMA 3.18 guarantees us the norm estimates

$$\begin{aligned} \|tr_x e\|_{H^1(I_t)} &= \|tr_x e\|^2_{H^1\left(I_x^{impl}\right)} + \|tr_x e\|_{H^1\left(I_x^{expl}\right)} \\ &\leq v^{max} \left\|e^{init}\right\|_{H^1\left(\Omega_0^{impl}\right)} + \frac{v^{max}}{v^{min}} \left\|e^{in}\right\|_{H^1\left(I_0^{impl}\right)} \\ &\leq v^{max} \left\|e^{init}\right\|_{H^1(\Omega)} + \frac{v^{max}}{v^{min}} \left\|e^{in}\right\|_{H^1(I_t)} \end{aligned} \tag{3.111}$$

such that tr_x is a linear and bounded operator for every $x \in \bar{\Omega}$. □

3.2 Well-posedness and regularity for networks without flow reversal

After this thorough analysis of the single pipeline problem, we are going to extend the results of SECTION 3.1 to slightly more complex networks, whose graph structure is a simple graph according to DEFINITION 2.6.
At first, we recognize that all pipelines in $\mathcal{A}_P^{ff}$, whose outflow is connected to a consumer, can be partially reduced to a single pipeline problem for a restricted time interval. This allows us to constructively extend the existence and uniqueness results with continuous data in SECTION 3.2.1, and improved regularity for H^1 data in SECTION 3.2.2.
Finally, we conclude the discussion about existence and uniqueness of solutions with the treatment of the hydraulic equations in SECTION 3.2.3.

3.2.1 Continuous solutions

We start the generalization of the results from SECTION 3.1 to simple networks with the following observation:

3.20 Lemma (Simplified coupling conditions in forward flow)

Let $\mathfrak{G}$ be the graph of a simple district heating network in accordance with definition DEFINITION 2.6. Then all quantities of the forward flow network $\mathfrak{G}^{ff}$ can be computed independently from those ones of the return flow, and $v_a > 0 \forall a \in \mathcal{A}_P$.
Furthermore, one can equivalently replace the energy balance equation by

$$e_n = e_{a:n}, o(a) = n, a \in \mathcal{A}_P^{ff}. \tag{3.112}$$

and conservation of volume

$$\sum_{a \in \mathcal{I}_n} q_{a:n}, n \in \mathcal{N}^{ff} \tag{3.113}$$

automatically implies conservation of mass for each node $n \in \mathcal{N}^{ff}$.

Proof. We rearrange the mass conservation equations for consumers and obtain

$$q_{c:in} = -\frac{\rho(\hat{e}_{i(c)})}{\rho(e_c^{ret})} q_{c:out} \tag{3.114}$$

such that $q_{c:in}$, and $q_{c:out}$ only differ by a negative scaling factor $s(e_{i(c)})$ with $\left|s(e_{i(c)})\right| < 1$, where $\hat{e} = \phi(e)$ is the regularized supply energy.
By using this expression in the energy balance equation

$$Q_c^{pred} = q_{c:out} \left(e_{i(c)} - \frac{e_c^{ret}}{\rho(e_c^{ret})} \rho(e_{i(c)}) \right) \tag{3.115}$$

we obtain

$$Q_{c:in} + Q_{c:out} = -q_{c:out} \left(\hat{e}_{i(c)} - e_c^{ret} \frac{\rho(\hat{e}_{i(c)})}{\rho(e_c^{ret})} \right), \tag{3.116}$$

and conclude, that all consumer fluxes do not depend on quantities defined on the return flow network. Next we show, that $v_a > 0 \forall a \in \mathcal{A}_P^{ff}$. By the monotonicity and boundedness

properties of ρ we get

$$\hat{e}_{i(c)} > e_c^{ret} > e_c^{ret} \frac{\rho(\hat{e}_{i(c)})}{\rho(e_c^{ret})} \tag{3.117}$$

such that $q_{c:in} < 0$ for each consumer. Given a pipeline a with $o(a) = i(c)$ for some $c \in \mathcal{A}_C$, we can define the set

$$\tilde{N}_0^{ff} = \left(\mathcal{N}^{ff} \cap \mathcal{N}^{ext}\right) \setminus n^{ff} \tag{3.118}$$

of interior nodes in the forward flow network, for which all outgoing mass fluxes are known. Right now, this set contains precisely those ones, which are connected to a consumer, such that we can immediately compute the flow velocity

$$v_a = -\frac{q_{c:in}}{A_a} > 0, \tag{3.119}$$

which is strictly positive. Due to DEFINITION 2.6, the forward flow network has a tree structure, and each node in $\mathcal{N}^{ff} \setminus \mathcal{N}ext$ is connected to pipes only, with $deg(n) \geq 2$. We recursively define

$$\tilde{N}_k^{ff} = \left\{ i(a) \,\middle|\, a \in \mathcal{A}_P^{ff} : o(a) \in \tilde{N}_{k-1}^{ff} \right\} \tag{3.120}$$

which is non-empty, as long there are any unknown flow velocities in $\mathcal{A}_P^{ff}$, such that we can explicitly compute

$$v_a = -\frac{\sum_{b \in \mathcal{I}(n) \setminus a} q_{b:n}}{d_a} > 0 \tag{3.121}$$

for all a with $o(a) \in \tilde{N}_k^{ff}$.
We repeat this process, until $\tilde{N}_k^{ff}$ becomes the empty set for the firs time. Now we can compute

$$q_{s:out} = -\sum_{b \in \mathcal{I}(n^{ff}) \setminus s} q_{b:n} > 0 \tag{3.122}$$

For the return flow network, we follow an analogous argument, such that we can summarize this result with

$$q_{a:out} > 0 \forall a \in \mathcal{A}. \tag{3.123}$$

Therefore, we know that the water flow does not change directions, and the perfect mixing condition for pipes simplifies to

$$Q_{a:in} = e_{i(a)} q_{a:in} \forall a \in \mathcal{A}_P^{ff} \cup \mathcal{A}_C \tag{3.124}$$

As there is only one component with $o(a) = n$ for every $n \in \mathcal{N}^{ff}$, which is either the producer, or a pipe, we can rearrange the node balance equations for energy

$$e_{a:n} q_{a:n} = -e_n \sum_{b \in \mathcal{I}(n) \setminus a} q_{b:n}, \tag{3.125}$$

and mass

$$\rho(e_{a:n}) q_{a:n} = -\rho(e_n) \sum_{b \in \mathcal{I}(n) \setminus a} q_{b:n}, \tag{3.126}$$

which yields the compatibility condition

$$\frac{e_{a:n}}{\rho(e_{a:n})} = \frac{e_n}{\rho(e_n)}. \tag{3.127}$$

Since we assume ρ to be bounded, and either constant or strictly decreasing, we see that $e_n = e_{a:n}$ is the only possible solution. In particular, we conclude that $e_{nff} = u^e$. Finally, conservation of mass becomes equivalent to

$$\sum q_{a:n} = 0, \forall n \in \mathcal{N}^{ff}, \tag{3.128}$$

as e is continuous across junctions. □

This result delivers a strategy, how to solve the energy transport problem for simple networks: Given a pipeline which is connected to a consumer's inlet, we already know how to (partially) solve the nonlocal advection problem. In particular, we can determine the flow velocity for all such pipelines within a certain subinterval of I_t, and extend this solution to all flow velocities and volume fluxes in $\mathfrak{G}^{ff}$.

3.21 Lemma

Let g be a bounded, positive, monotonously decreasing function, and f Lipschitz and bounded. Then $h(x)\frac{f(x)}{g\circ f(x)}$ is Lipschitz as well.

Proof. Without loss of generality, assume that $f(x) < f(y)$, and define $g^{min} = g(f^{min})$.

$$\begin{aligned} \|h(x) - h(y)\|_\infty &= \left\| \frac{f(x)}{g \circ f(x)} - \frac{f(y)}{g \circ f(y)} \right\|_\infty \\ &\leq \left\| \frac{f(x) - f(y)}{g \circ f(y)} \right\|_\infty \leq L_f \frac{\|x - y\|_\infty}{g^{min}} \end{aligned} \tag{3.129}$$

□

Unlike in the single pipeline case, the compatibility of the initial energies e_a^{init} with the nodal energies $e_n(t_0)$ at the initial time point is not enough to ensure the existence of continuous solutions. In addition, we have to consider the flux coupling conditions

$$\begin{aligned} \sum_{a \in I_n} \rho\left(e_{a:n}\right)(t_0) q_{a:n}(t_0) = 0 \\ \sum_{a \in I_n} Q_{a:n}(t_0) = 0, \end{aligned} \tag{3.130}$$

at the time t_0. Now we can formulate the regularity assumptions for continuous solutions of simple district heating networks as follows:

Assumption 3.22: Regularity assumptions for C^0 solutions

C.1 The initial values $e_a^{init} \in C^0(\bar{\Omega}_a)$ are bounded by $e^{min} \leq e_a^{init} \leq e^{max}$, and satisfy $e_a(t_0)(0) = e_{i(a)}(t_0)$ for all $a \in \mathcal{A}_P$.

C.2 The control input $u_s^e \in C^0(\bar{I}_t)$ with $u_s^{e,min} \leq u_s^e \leq u_s^{e,max}$. Further $u_s^e(t_0) = e_{o(s)}(t_0)$.

C.3 All node energies e_n and fluxes $q_{a:n}, Q_{a:n}$ are consistent with the coupling conditions (3.130) at the time t_0 for all $n \in \mathcal{N}, a \in \mathcal{A}$.

C.4 The consumer return energies satisfy $e^{wall} < e_c^{ret} < e^{e,min} \leq e^{max}$ for all $c \in \mathcal{A}_C$.

C.5 The consumption prediction models $\Delta Q_c^{pred} \in C^0(\bar{I}_t)$ are positive, bounded functions, such that $0 < \Delta Q_c^{min} \leq \Delta Q_c^{pred} \leq \Delta Q_c^{max}\ \forall c \in \mathcal{A}_C$.

C.6 $e^{ret} < u^{e,min} \leq e^{e,min} \leq e^{max} \leq u^{e,max}$

3.23 Theorem (Continuous solution for tree shaped networks)

Let $\mathfrak{G}$ be the graph of simple district heating network in compliance with definition DEFINITION 2.6*. Further, let ΔQ_c^{pred}, u^e, and $e_{init,a}$ which fulfil* ASSUMPTION 3.22*. Then the system* (2.94)-(2.103)*, excluding inequalities and all equations involving the hydraulic pressure, has a unique continuous solution in the sense that $e_a \in C^0(\bar{I}_t \times \bar{\Omega}_a)$ is a generalized solution of the advection problem in terms of* PROPOSITION 3.3*, and all other state variables are continuous and bounded on $\bar{I}_t$.*

Proof. According to LEMMA 3.20, it is sufficient to focus on the forward flow network at first. Consider the set $\tilde{\mathcal{A}}_P$ of all pipelines $a \in \mathcal{A}_P^{ff}$, with $o(a) = i(c)$ for some consumer $c \in \mathcal{A}_C$.
By assumption, there exists a pipeline $a \in \mathcal{A}_P^{ff}$, such that

$$e_{c:in} \coloneqq \phi_c(e_{i(c)}) = \phi_c(e_a(\cdot, L_a)) \tag{3.131}$$

is Lipschitz continuous with respect to $e_{i(c)}$ and e_a. We use the relation

$$q_{a:out} = v_a A_a = -q_{c:in} \tag{3.132}$$

within the consumer's energy balance equation

$$\Delta Q_c^{pred} = v_a A_a \left(\frac{e_{c:in}}{\rho(e_{c:in})} \rho(e_c^{ret}) - e_c^{ret} \right) \tag{3.133}$$

and obtain the expression

$$v_a = \frac{\Delta Q_c^{pred}}{A_a \left(\frac{e_{c:in}}{\rho(e_{c:in})} \rho(e_c^{ret}) - e_c^{ret} \right)} \tag{3.134}$$

which is Lipschitz according to lemma 3.2.1.
Further, we can estimate an upper bound for the flow velocities of all pipelines

$$v_a^{max} = \frac{\left\| \Delta Q_c^{pred} \right\|_\infty}{A_a \left(\frac{e^{min}}{\rho(e^{min})} \rho(e_c^{ret}) - e_c^{ret} \right)} \tag{3.135}$$

such that there the outflow trace $e_a(t, L_a)$ only depends on e_a^{init}, whenever $t \in \left[t_0, t_0 + \frac{L_a}{v_a^{max}}\right]$. We define Δt^{exp} as the largest possible time step, such that this assertion holds for all pipelines, which are directly connected to a consumer. Therefore, we effectively reduced the problem to the case of a single consumer network, such that COROLLARY 3.12 guarantees the existence and uniqueness of a continuous solution for each such pipeline.
By LEMMA 3.20 we already know, that all remaining flow velocities are computable, positive, and bounded. For the solution of the remaining pipelines $a \in \mathcal{A}_P^{ff}$, we traverse the forward flow network in orientation preserving order, starting with the root node n^{ff}.
We define the set

$$\mathcal{N}_k = \left\{ o(a) \,\middle|\, a \in \mathcal{A}_P^{ff} : i(a) \in \mathcal{N}_{k-1} \right\}, \quad k > 0 \tag{3.136}$$

of nodes, which are computable at step k, which we initialize with

$$\mathcal{N}_0 = \{n^{ff}\}. \tag{3.137}$$

For each node $n \in \mathcal{N}_k$, we apply COROLLARY 3.12 to all pipes with $i(a) = n$. This is always possible, since $e_{n^{ff}} = u^e$, and each pipeline $a \in \mathcal{A}_P^{ff}$ has successor node, and the traversal process continues, until every consumer has been reached. Analogously to the single pipeline problem, we repeat this procedure until the entire time domain $\bar{I}_t$ has been covered.
For the return flow network we use a similar induction argument, where we traverse the graph starting with the nodes located at the consumer's outlets.

$$\mathcal{N}_0 = \left\{ o(c) \,\middle|\, c \in \mathcal{A}_C \right\} \tag{3.138}$$

$$e_{c:n} = e_c^{ret}, \qquad q_{c:out} = -\frac{\rho(e_{c:in})}{\rho(e_c^{ret})} q_{c:in} \tag{3.139}$$

By the definition of *simple networks*, for every $n \in \mathcal{N}_0$ (and $\mathcal{N}^{rf}$ in general), there exists exactly one edge $a_0 \in \mathcal{A}^{rf}$ such that $I^-(n) = \{a_0\}$. We rearrange the conservation laws for mass and energy

$$\sum_{a \in I^+(n)} e_{a:n} q_{a:n} + e_n q_{a_0:n} = 0 \tag{3.140a}$$

$$\sum_{a \in I^+(n)} \rho(e_{a:n}) q_{a:n} + \rho(e_n) q_{a_0:n} = 0 \tag{3.140b}$$

and obtain

$$\begin{aligned} e_n &= \rho(e_n) \frac{\sum_{a \in I^+(n)} e_{a:n} q_{a:n}}{\sum_{a \in I^+(n)} \rho(e_{a:n}) q_{a:n}} \\ &= \rho(e_n) \cdot f, \end{aligned} \tag{3.141}$$

where the functions determining f are always known, when the node n is traversed. By the definition of f, and the monotonicity properties of ρ, we know that

$$\frac{e^{min}}{\rho(e^{min})} \leq f \leq \frac{e^{max}}{\rho(e^{max})} \tag{3.142}$$

and

$$e^{min} \leq \rho(e_n) \cdot f \leq e^{max} \tag{3.143}$$

hold, such that the equation must have a unique solution. Here we emphasise, that ρ was assumed to be strictly positive and nowhere increasing, such that it cannot be a linear function. Therefore, the set of conservation laws (3.140) is never redundant.
Now, we define the set

$$\mathcal{N}_1 = \left\{ n \in \mathcal{N}^{rf} \,\middle|\, i(a) \in \mathcal{N}_0 \forall a \in I^+(n) \right\} \tag{3.144}$$

of all nodes, whose inflow variables are computable during the first iteration of the graph traversal. Due to the topology of the return flow network it may occur, that only a subset of the edges in $I^-(n)$ directed towards a node $n \in \mathcal{N}^{rf}$ are computable. We introduce the sets

$$\mathcal{M}_0 = \{\}\,, \tag{3.145a}$$

$$\mathcal{M}_k = \left(\left\{ o(a) \,\middle|\, n \in \mathcal{N}_{k-1} \cup \mathcal{M}_{k-1}, a \in I^-(n) \cap \mathcal{A}_P \right\} \cup \mathcal{M}_{k-1} \right) \setminus \mathcal{N}_k, \quad k > 0, \tag{3.145b}$$

which contain all nodes which have not been traversed yet, even though their average energy can be computed. Finally, we define the set of nodes

$$\mathcal{N}_k = \left\{ n \in \mathcal{N}^{rf} \,\middle|\, i(a) \in \mathcal{N}_{k-1} \cup \mathcal{M}_{k-1} \forall a \in I^+(n) \right\}, \quad k > 0, \tag{3.146}$$

which are computable during the k^{th} iteration.
Now we repeatedly solve the equations for all pipelines with $i(a) \in \mathcal{N}_k$, and update the sets $\mathcal{N}_{k+1}, \mathcal{M}_{k+1}$, until we reach the first iteration $\hat{k}$, such that $\mathcal{N}_{\hat{k}} = \{\}$. By assumption, the return flow pipe network $\left(\mathcal{N}^{rf}, \mathcal{A}_P^{rf}\right)$ has the topology of an inverted tree, where the root node is located at the producer's inlet. In particular, every node $n \in \mathcal{N}^{rf}$ is reachable by a unique path, starting at a consumer's outlet, such that $\mathcal{K}_{\hat{k}}$ must be empty, and all nodes in $\mathcal{N}^{rf}$ have been traversed.

□

3.2.2 Continuous solutions with data in H^1

We extend the improved existence, uniqueness, and regularity results for the nonlocal advection problem to simple networks. An equivalent statement for the forward flow sub-network directly follows from the one dimensional case. For the return flow network, the node energies e_n are defined as the weighted averages

$$e_n = -\frac{\sum_{a \in I_n^+} e_{a:n} q_{a:n}}{\sum_{a \in I_n^-} q_{a:n}} \tag{3.147}$$

of all incoming energy fluxes.
In the special case, that all $e_{a:n}$, and outgoing fluxes $q_{a:n}, a \in I_n^-$, are constant in time, we immediately see that $e_n \in H^1(I_t)$, if and only if $q_{a:n} \in H^1(I_t) \forall a \in I_n^+$. Therefore, we need to specify additional conditions, under which all volume fluxes are weakly differentiable.
In the proof of THEOREM *3.23* we have seen, that all volume fluxes (and flow velocities) are uniquely defined, once equations of the feed forward network have been solved. As pointed out in COROLLARY *3.8*, we can derive C^1 estimates for v (and therefore q), if the consumer demand functions are continuously differentiable. The generalized quotient rule for Sobolev spaces REMARK *3.17* allows us to extend this result to weakly differentiable data, if assume the following:

Assumption 3.24: Extended Regularity assumptions for C^0 solutions with H^1 data

In addition to ASSUMPTION 3.22, we assume the following:

C.1′ $e_a^{init} \in H^1(\Omega_a)$ for all $a \in \mathcal{A}_P$.

C.2′ $u_s^e \in H^1(I_t)$.

C.4′ $\Delta Q_c^{pred} \in H^1(I_t)$ for all $c \in \mathcal{A}_C$

The improved regularity result for data in H^1 follows immediately:

3.25 Corollary (Existence and uniqueness of solutions for simple networks with data in H^1)

Let $(\mathcal{N}, \mathcal{A})$ be the DEFINITION 2.6 *and let all initial and boundary data be compliant with* ASSUMPTION 3.24*. Then the continuous solution given in* THEOREM 3.23 *admits higher regularity. In particular, the state variables v_a, $q_{a:n}$, $Q_{a:n}$, e_n are all elements of $H^1(I_t)$, and the energy densities admit continuous representatives with weak spatial derivatives $e_a \in C^0\left(\bar{I}_t, H^1(\Omega_a)\right)$, such that the point evaluation $tr_{a,x} e_a \in H^1(I_t)$ is weakly differentiable for all $x \in \bar{\Omega}_a$.*

Proof. For the forward flow network, we slightly alter the proof of THEOREM 3.23, and apply the regularity result THEOREM 3.19 for each pipeline.
The representatives in $C^0\left(\bar{I}_t, H^1(\Omega_a)\right)$ guarantee that the explicit time stepping argument is compatible with ASSUMPTION 3.24. For the improved regularity of all state variables without a spatial component, we apply the results LEMMA 3.14 (product rule in H^1), LEMMA 3.16 (chain rule), and REMARK 3.17 (quotient rule).
For the return flow network, we have to take a closer look onto the coupling conditions, As in the proof of THEOREM 3.23 we observe, that for every node $n \in \mathcal{N}^{rf}$, the outflow incidence set consist of a single element $I^-(n) = \{a_0\}$. We use REMARK 3.17 to explicitly compute the weak derivative

$$\partial_t e_n = -\frac{\sum_{a \in I_n^+} \partial_t e_{a:n} q_{a:n} + e_{a:n} \partial_t q_{a:n}}{q_{a_0:n}} + \frac{\left(\sum_{a \in I_n^+} e_{a:n} q_{a:n}\right) \partial_t q_{a_0:n}}{\left(q_{a_0:n}\right)^2} \tag{3.148}$$

such that we can safely apply THEOREM 3.19 to get the desired regularity result for e_a with $a \in \mathcal{A}_P^{rf}$. □

Remark 3.26: Nonlocality in simple district heating networks

We observe two fundamental differences between the dynamical behaviour of the forward and return flow networks.
As we have already pointed out in the introduction of this chapter, the single-pipeline model can be interpreted as a nonlocal advection problem, where the flow velocity is determined by the trace $tr_L e$ at the outflow boundary. The same reasoning holds true for the forward flow of simple district heating network, where the flow behaviour is uniquely determined by the outflow traces $tr_{L_a} e_a$ of all pipelines, which are directly connected to a consumer. As a consequence, every change of the initial conditions or model parameters (length, diameter, ...) of any pipeline $a \in \mathcal{A}_P^{ff}$ can potentially

affect every other state variable in the entire forward flow network.
This is not true for the return flow network, where all information travels strictly downstream.

3.2.3 Solutions of the hydraulic system with controls in H^1

So far, we have mostly dealt with the thermodynamic part of the equation system, which we have derived in CHAPTER 2, as the hydraulic pressure is not needed in order to fully describe the advective energy transport of simple networks. Given a solution $(v_a, ea)_{a\in\mathcal{A}_P}$ of the advection system, we can rearrange (2.94b), and immediately compute the pressure

$$p_{o(a)}(t) = p_{i(a)}(t) - \left(g\frac{\Delta h_a}{L_a} + \frac{\lambda_a}{2d_a}v_a(t)\,|v_a(t)|\right)\int_{\Omega_a}\rho\,(e_a)\,(t)(x)\,dx \tag{3.149}$$

at the outflow boundary of a pipeline $a \in \mathcal{A}_P^{ff}$, if we assume that the pressure $p_{i(a)}$ at the inflow boundary is already known. A similar argument holds for all pipelines in the return flow network. We propose the following regularity assumptions

Assumption 3.27: C^0 regularity assumptions for hydraulic control variables

In addition to ASSUMPTION 3.22 we require that

H.1 The networks reference pressure is a continuous function $u^{p_0} \in C^0\big(\bar{I}_t\big)$ with $u^{p,min} \le u^{p_0} \le u^{p,max}$.

H.2 The pressure difference between forward and return flow is a continuous function $u^{\Delta p} \in C^0\big(\bar{I}_t\big)$ with $0 < u^{\Delta p,min} \le u^{\Delta p} \le u^{\Delta p,max}$.

for continuous solutions of the complete thermohydraulic system. If more regularity is needed, we additionally require that

Assumption 3.28: H^1 regularity assumptions for hydraulic control variables

In addition to ASSUMPTION 3.27 and ASSUMPTION 3.24, we require that

H.1′ $u^{p_0} \in H^1(I_t)$,

H.2′ $u^{\Delta p} \in H^1(I_t)$, and

H.3′ ρ is Lipschitz continuous.

3.29 Proposition (Solution of the hydraulic pressure equations for simple DHN)

Let $(\mathcal{N}, \mathcal{A})$ be a the graph representation of a district heating network, and assume that ASSUMPTION *3.27 is fulfilled.*
Then the hydraulic pressure is uniquely defined by (2.94b) and has a continuous representative. In particular, the estimates

$$p_{o(a)}^{min} \geq p_{i(a)}^{min} - \left(g\frac{\Delta h_a}{L_a} + \frac{\lambda_a}{2d_a} v_a^{max} \left| v_a^{max} \right| \right) L_a \rho \left(e_a^{min} \right) \tag{3.150}$$

and

$$p_{o(a)}^{max} \leq p_{i(a)}^{max} - \left(g\frac{\Delta h_a}{L_a} + \frac{\lambda_a}{2d_a} v_a^{min} \left| v_a^{min} \right| \right) L_a \rho \left(e_a^{max} \right) \tag{3.151}$$

hold for every pipeline $a \in \mathcal{A}_P$, where e_a^{min} and e_a^{max} denote the respective spatial minima and maxima.
If additionally ASSUMPTION *3.28 is fulfilled, the nodal pressures satisfy $p_n H^1(I_t)$ for each node $n \in \mathcal{N}$.*

Proof. By THEOREM *3.23* the energy densities e_a and flow velocities v_a are continuous, positive, bounded functions. Furthermore, ρ is a non-negative, continuous function, such that the first statement, including the estimates (3.150) and (3.151), immediately follows.
If ASSUMPTION *3.28* is fulfilled, the weak differentiability of all p_n is a consequence of COROLLARY *3.25*, paired with the generalized chain rule LEMMA *3.16*. □

Remark 3.30: Worst case estimates of the pressure differences at consumer stations

In analogy to REMARK *3.13*, we can derive rough estimates for the propagation of hydraulic pressure throughout the network. Let $P_c^+ = (a_0^+, \dots, a_{k_c}^+)$ be the unique path of pipelines connecting the outflow of the source with the inflow of a consumer $c \in \mathcal{A}_C$. Then a repeated application of the estimates (3.150) and (3.151) yields

$$p_{i(c)}^{min} \geq u^{p,min} + u^{\Delta p,min} - \sum_{a \in P_c^+} \left(g\frac{\Delta h_a}{L_a} + \frac{\lambda_a}{2d_a} v_a^{max} \left| v_a^{max} \right| \right) L_a \rho \left(e_a^{min} \right) \tag{3.152}$$

and

$$p_{i(c)}^{max} \leq u^{p,max} + u^{\Delta p,max} - \sum_{a \in P_c^+} \left(g\frac{\Delta h_a}{L_a} + \frac{\lambda_a}{2d_a} v_a^{min} \left| v_a^{min} \right| \right) L_a \rho \left(e_a^{min} \right) \tag{3.153}$$

for each consumer. In the same way, along each orientation preserving path $P_c^- = (a_0^-, \dots, a_{k_c}^-)$ in the return flow network, which connects a consumer's outlet with the producers inflow, we obtain the estimates

$$p_{o(c)}^{min} \geq u^{p,min} + \sum_{a \in P_c^-} \left(g\frac{\Delta h_a}{L_a} + \frac{\lambda_a}{2d_a} v_a^{max} \left| v_a^{max} \right| \right) L_a \rho \left(e_a^{min} \right) \tag{3.154}$$

and

$$p_{o(c)}^{max} \leq u^{p,max} + \sum_{a \in P_c^-} \left(g\frac{\Delta h_a}{L_a} + \frac{\lambda_a}{2d_a} v_a^{min} \left| v_a^{min} \right| \right) L_a \rho \left(e_a^{min} \right), \tag{3.155}$$

such that we can compute the bounds

$$\Delta p_c^{min} \leq p_{o(c)}^{max} - p_{i(c)}^{min}, \tag{3.156}$$
$$\Delta p_c^{max} \leq p_{o(c)}^{min} - p_{i(c)}^{max}, \tag{3.157}$$

for the pressure difference at each consumer stations. The sharpness of each estimate heavily depends on the respective path length between the source and each consumer station, as well as the variation of energies e_a and flow velocities v_a.

This concludes our studies of continuous solutions of the model equations for simple district heating networks networks with data in H^1. In the next section, we are going to build upon these results, in order to construct an abstract formulation of the governing equations, which is suitable for applications in optimization.

3.3 Weak formulation and analysis of the residual operator $\mathcal{G}$

In SECTION 3.1.4 we have shown, that the solution of the IBVP for a single pipeline is an element of $C^0\big(I_t, H^1(\Omega)\big)$, if the initial and boundary data are compatible, and regular enough. The Banach-valued version of e is simply defined as the partial evaluation

$$e(t) = e(t, \cdot) \tag{3.158}$$

at a time point t.
Using the Riesz-Fréchet isomorphism $R_{L^2} : L^{2\star} \to L^2$, and the (continuous and closed) inclusion map $i^\star : L^{2\star} \to H^{1\star}$, we can identify the expression

$$\partial_t e(t,x) = -v(t)\partial_x e(t,x) - r(e(t,x) = -v(t)\left(\partial_x e(t)\right)(x) - r(e)(t)(x) \tag{3.159}$$

with a linear functional $\phi_{\partial_t e(t)} \in H^1(\Omega)^\star$, which we define as

$$\left\langle \phi_{\partial_t e(t)}, \omega \right\rangle_{H^1(\Omega)^\star, H^1(\Omega)} \coloneqq \left\langle i^\star R_{L^2}^{-1} \partial_t e(t), \omega \right\rangle_{H^1(\Omega)^\star, H^1(\Omega)} \tag{3.160}$$
$$= \left(-v(t)\partial_x e(t), \omega\right)_{L^2(\Omega)} \tag{3.161}$$

for every $t \in I_t$, and $\omega \in H^1(\Omega)$.
Since all mapping involved in this identification are linear and continuous, we can formally define the Banach-valued time derivative

$$\frac{d}{dt} e(t) \coloneqq \phi_{\partial_t e(t)} \in C^0\big(I_t, H^1(\Omega)^\star\big) \tag{3.162}$$

and

$$\mathcal{E} \coloneqq C^1\big(I_t, H^1(\Omega), H^1(\Omega)^\star\big), \tag{3.163}$$

the space of continuous, H^1 valued functions, whose derivative is continuous and takes values in $H^{1\star}$, becomes a candidate for the co-domain of the advection's residual operator $\mathcal{G}^{adv}$. Unfortunately, the corresponding dual space, consisting of vector valued Borel measures, is too large for our purpose, and the resulting weak formulation

$$\left\langle \mu, \mathcal{G}^{adv}(e) \right\rangle_{\mathcal{B}(I_t, H^1(\Omega)), C^0(I_t, H^1(\Omega)^\star)} = \int_{I_t} \mathcal{G}(e)(t) d\mu(t) \tag{3.164}$$

lacks the desired symmetry.
If we relax the continuity assumption for the derivative, such that

$$\frac{d}{dt}e(t) \in H^1(\Omega)^\star \qquad \text{for a.e. } t \in I_t, \tag{3.165}$$

we hope to rewrite (3.164) in terms of a scalar product, which satisfies all of the continuity and differentiability properties, which are needed in the context of optimization problems. Starting with the formal identity

$$\int_{I_t} \left\langle \frac{d}{dt}e(t), \omega(t) \right\rangle_{H^1(\Omega)} dt := -\int_{I_t} \left(v(t)\partial_x e(t) + r\left(e\right)(t), \omega(t)\right)_{L^2(\Omega)} dt, \tag{3.166}$$

we are going to construct a vector valued residual operator, whose solution set is equivalent to the one specified in SECTION 3.2. Note, that we have yet to rigorously define appropriate function spaces for e and ω.

3.3.1 Construction of $\mathcal{G}$ in (generalized) Sobolev spaces

3.31 Definition (Bochner space [Schweizer, 2013])

Given a measure space $(I, \mathfrak{S}, \mu)$, and a Banach space $(X, \|\cdot\|_X)$ we call a function $f : I \to X$ Bochner measurable*, if there exists a sequence $(f_n)_n$ of* finite valued functions

$$f_n(t) = \sum_{k=0}^{M} f_{n,k}\chi_{I_{n,k}}(t) \tag{3.167}$$

with $f_{n,k} \in X$, and $I = \bigcup_{k=0}^{M} I_{n,k}$, such that

$$f(t) = \lim_{n\to\infty} f_n(t) \text{ for } \mu \text{ almost every } t. \tag{3.168}$$

Using the norms

$$\|f\|_{L^p I,X} := \left(\int_I \|f(t)\|_X^p \, d\mu(t)\right)^{\frac{1}{p}}, \qquad 1 \le p < \infty \tag{3.169}$$

and

$$\|f\|_{L^\infty I,X} := \operatorname*{ess\,sup}_{t\in I} \|f(t)\|_X \tag{3.170}$$

we define the sets

$$\mathcal{L}^p(I,X) := \left\{ f : I \to X \;\middle|\; f \text{ is Bochner measurable and } \|f\|_{L^p I,X} < \infty \right\} \tag{3.171}$$

and the Bochner spaces $L^p(I,X)$ as the set of equivalence classes of functions in $\mathcal{L}^p(I,X)$ which μ-a.e. identical.

We emphasize a particular property of the Bochner integral, which we are going to use in later proofs.

3.32 Theorem (Bochner integral)

Let $(I, \mathfrak{S}, \mu)$ be a measure space, $(X, \|\cdot\|_X)$ a Banach space, and $p > 0$. For any function $f \in L^p(I, X)$, the Bochner integral satisfies

$$\left\| \int_I f(t)\, dt \right\|_X \leq \int_I \|f(t)\|_X \, dt, \tag{3.172}$$

and

$$\left\langle \phi, \int_I f(t)\, dt \right\rangle = \int_{I_t} \langle \phi, f(t) \rangle \, dt \forall \phi \in X^\star. \tag{3.173}$$

Proof. For the full version of the theorem, covering well-posedness, approximation by finite valued functions, and a generalized Lebesgue convergence theorem, and a proof, we refer to *Theorem 10.4*, [Schweizer, 2013]. □

The Bochner-measurability of a function can be hard to prove at some times. In the case, that an abstract function maps into a separable Banach space, this strong measurability property can be relaxed significantly:

3.33 Theorem (Pettis)

Let $(I, \mathfrak{S}, \mu)$ be a measure space, and $(X, \|\cdot\|_X)$ a Banach space. Then $f : I \to X$ is Bochner measurable, if and only if :

- *f is* weakly measurable*, i.e. $\langle x^\star, f(t) \rangle_{X^\star, X}$ is Lebesgue measureable for every $x^\star \in X^\star$, and for μ-almost every t.*
- *It is μ-almost surely separably valued.*

Proof. See [Schweizer, 2013] □

In the following, we are going to assume that $(I, \mathfrak{S}, \mu)$ refers to the standard Lebesgue measure space over a real interval I, and write dt instead of $d\mu(t)$.
Following the result THEOREM *3.19* from SECTION *3.1*, we already know that

$$e \in C^0\big(I_t, H^1(\Omega)\big) \tag{3.174}$$

such that we can conclude

$$e \in L^2\big(I_t, H^1(\Omega)\big) \tag{3.175}$$

as a consequence of THEOREM *3.33*. Next, we would like to generalize the time derivative of e in such a way that it preserves some of the nice geometrical properties of the Bochner space $L^2\big(I_t, H^1(\Omega)\big)$.

3.34 Definition (Geldfand triple)

Let $(H, (\cdot, \cdot)_H)$ be a Hilbert space, and $(V, \|\cdot\|_V)$ a Banach space, such that the inclusion map $i : V \to H$ is continuous and dense, and $i^\star : H^\star \to V^\star$ is continuous. Then the tuple $(V, H, V^\star)$ is called ***Gelfand triple****.*

As pointed out in the introduction of this chapter, we can interpret the action of the (partial) time derivative

$$\partial_t e(t) = -v(t)\partial_x e(t) - r(e)(t) \tag{3.176}$$

as a linear functional over $H^1(\Omega)$ for almost every t. This motivates the choice of *generalized Sobolev spaces*, which are commonly used in the context of weak formulations of the heat equations, as the appropriate function space for the energy densities e_a.

3.35 Definition (Weak derivatives, generalized Sobolev spaces, and Gelfand triples)

Let $(X, \|\cdot\|_X)$ be a Banach space and $f \in L^1(I, X)$. Then f is said to be weakly differentiable*, if there exists $g \in L^1(I, X)$*

$$\int_I f(t)\phi'(t)\,dt = -\int_I g(t)\phi(t)\,dt \qquad \forall \phi \in C_0^\infty(I) \tag{3.177}$$

and call $\frac{d}{dt}f = g$ the weak (time) derivative *of f.*
We define the vector valued Sobolev spaces *as the set of functions*

$$W^{1,p}(I, X) \coloneqq \left\{ f \in L^p(I, X) \,\middle|\, f \text{ is weakly differentiable and } \frac{d}{dt}f \in L^p(I, X) \right\}, \tag{3.178}$$

which we equip with the norm

$$\|f\|_{W^{1,p}(I,X)} \coloneqq \sqrt{\|f\|^2_{L^p(I,X)} + \left\|\frac{d}{dt}f\right\|^2_{L^p(I,X)}}. \tag{3.179}$$

In the case, that X is a Hilbert space, we write $H^1(I, X) \coloneqq W^{1,2}(I, X)$.
Let $(H, (\cdot,\cdot)_H)$ be a Hilbert space, such that the inclusion map *$i : X \to H$ is continuous and dense, and the relations $X \subset H \subset X^\star$ hold in the sense that*

$$X \underset{i}{\to} H \underset{R_H^{-1}}{\to} H^\star \underset{i^\star}{\to} X^\star, \tag{3.180}$$

where $R_H : H^\star \to R_H$ is the Riesz isomorphism. We define the generalized Sobolev space *as*

$$H^1(I, X, X^\star) \coloneqq \left\{ f \in L^2(I, X) \,\middle|\, f \text{ is weakly differentiable and } \frac{d}{dt}f \in L^2(I, X^\star) \right\} \tag{3.181}$$

equipped with the norm

$$\|f\|_{H^{I,X,X^\star}} \coloneqq \sqrt{\|f\|^2_{L^2(I,X)} + \left\|\frac{d}{dt}f\right\|^2_{L^2(I,X^\star)}}. \tag{3.182}$$

3.36 Theorem (C^0 representatives for Gelfand triples)

Let $(V, \|\cdot\|_V)$ be a Banach space, $(H, (\cdot,\cdot)_H)$ a Hilbert space, and $(V, H, V^\star)$ a Gelfand triple. Then the embedding $H^1(I_t, V, V^\star) \hookrightarrow C^0\big(\bar{I}_t, H\big)$ is continuous.

Proof. See [Hinze et al., 2009]. □

Before we can formulate an abstract residual operator for the full system, we have to address a technical difficulty, which arises when we try to generalize the notion of boundary conditions. For functions in $C^0\big(I_t, H^1(\Omega)\big)$ the point evaluation $tr_x e(t) = e(t)(x)$ is well defined, and even defines a mapping into $H^1(I_t)$ in the setting of COROLLARY 3.25. The additional regularity property is crucial, if we want to forward the solution of a pipeline to its adjacent ones, such that we require it to hold for the solution of $\mathcal{G}(\mathbf{u}, \mathbf{y}) = 0$.
For an arbitrary function f in $H^1\big(I_t, H^1(\Omega), H^1(\Omega)^\star\big)$, its trace $tr_x f$ can only be expected to be identified with an element of $L^2(I_t)$, but not $H^1(I_t)$. Fortunately, this is sufficient, because we intend to construct the residual operator as a mapping from $\mathcal{U} \times \mathcal{Y}$ with values in $\mathcal{Z} \subset \mathcal{Y}^\star$.
By using a construction involving a Gelfand triple (H^1, L^2, H^1), we can define a generalized trace operator

$$tr_x : H^1\big(I_t, H^1(\Omega), H^1(\Omega)^\star\big) \to L^2(I_t) \hookrightarrow H^1(I_t)^\star \tag{3.183}$$

such that the residual formulation of the inflow boundary condition

$$e_{a:in} - e_{i(a)} = tr_0 e_a - e_{i(a)} \in H^1(I_t)^\star \tag{3.184}$$

is well defined.

3.37 Lemma (Trace operator for generalized Sobolev spaces)

Let $I \subset \mathbb{R}$ be an open, real interval, and $y \in L^2\big(I_t, H^1(\Omega)\big)$. Then the trace operator $tr_x^H : H^1(\Omega) \to \mathbb{R}$ continuously extends to an operator

$$\begin{aligned} tr : \bar{\Omega} \times L^2\big(I_t, H^1(\Omega)\big) &\longrightarrow L^2(I_t) \\ (x, y(t)) &\longmapsto y(t)(x) \forall t \in I \end{aligned} \tag{3.185}$$

such that the point evaluation is well defined for this class of Bochner spaces.

Proof. Let $x \in \bar{\Omega}$ be arbitrary but fixed.
For any function $f \in L^2\big(I_t, H^1(\Omega)\big)$, the point evaluation operator tr_x^H defines a continuous, linear functional. By THEOREM 3.32, we can extend this operator family to an operator

$$\left\langle tr_x, \int_{I_t} f(t)\, dt \right\rangle \coloneqq \int_{I_t} \left\langle tr_x^H, f(t) \right\rangle dt \tag{3.186}$$

such that

$$tr_x : L^2\big(I_t, H^1(\Omega)\big) \to L^2(I_t). \tag{3.187}$$

Since $H^1(\Omega)$ is continuously embedded into $C^0(\Omega)$, there exists a constant $C_0 > 0$ independent of f, such that

$$\left\| tr_x^H f(t) \right\|_\infty \leq C_0 \left\| f(t) \right\|_{H^1(\Omega)} \tag{3.188}$$

holds for almost every $t \in I_t$.
This directly leads us to the norm estimates

$$\begin{aligned} \left\| tr_x^H f \right\|_{L^2(I_t)}^2 &= \int_{I_t} |\langle tr_x, f(t) \rangle|^2 \, dt \\ &\leq \int_{I_t} \|f(t)\|_\infty^2 \, dt \\ &\leq C_0^2 \int_{I_t} \|f(t)\|_{H^1(\Omega)}^2 \end{aligned} \tag{3.189}$$

such that tr_x is indeed bounded, and therefore continuous. □

Before we move to the formal definition of the full residual operator $\mathcal{G}$, we prove a small lemma, which is going to be useful in SECTION 3.3.2.

3.38 Lemma (Weak-weak* continuity of tr_x^H)

Let $(f_n)_n$ be a weakly convergent sequence of functions in $H^1\big(I_t, H^1(\Omega), H^1(\Omega)^\star\big)$. Then tr_x is continuous under weak convergence for every $x \in \bar{\Omega}$.

Proof. We need to show that

$$\langle tr_x f_n, g \rangle \to \langle tr_x f, g \rangle \, \forall g \in H^1(I_t). \tag{3.190}$$

According to LEMMA 3.37, the operator tr_x is linear and bounded, such that

$$\langle f_n, \tilde{g} \rangle = \langle tr_x f_n, g \rangle \tag{3.191}$$

defines a linear functional $\tilde{g} \in H^1\big(I_t, H^1(\Omega), H^1(\Omega)^\star\big)^\star$.
It immediately follows, that $tr_x f_n \rightharpoonup tr_x f$ weakly in $H^1(I_t)^\star$. □

Finally, we can begin with the (formal) construction of the residual operator $\mathcal{G}$. We start with the formulation of an appropriate state space.
For each pipeline $a \in \mathcal{A}_P$, we define function spaces

$$e_a \in H^1\big(I_t, H^1(\Omega_a), H^1(\Omega)^\star\big) =: \mathcal{E}_a \tag{3.192a}$$
$$v_a \in H^1(I_t) =: \mathcal{V}_a \tag{3.192b}$$
$$q_{a:in} \in H^1(I_t) =: \mathcal{M}_a^{in} \tag{3.192c}$$
$$q_{a:out} \in H^1(I_t) =: \mathcal{M}_a^{out} \tag{3.192d}$$
$$Q_{a:in} \in H^1(I_t) =: \mathcal{Q}_a^{in} \tag{3.192e}$$
$$Q_{a:out} \in H^1(I_t) =: \mathcal{Q}_a^{out} \tag{3.192f}$$

such that we can define the component state space of a as the cartesian product

$$\begin{aligned} \mathcal{Y}_a &= \mathcal{E}_a \times \mathcal{V}_a \times \mathcal{P}_a \times \mathcal{M}_a^{in} \times \mathcal{M}_a^{out} \times \mathcal{Q}_a^{in} \times \mathcal{Q}_a^{out} \\ &\cong \mathcal{E}_a \times \left(H^1(I_t)\right)^5, \end{aligned} \tag{3.193}$$

and the collective state of all pipelines as the cartesian product

$$\mathcal{Y}_{\mathcal{A}_P} = \prod_{a \in \mathcal{A}_P} \mathcal{Y}_a \cong \left(H^1(I_t)\right)^{5 \cdot |\mathcal{A}_P|} \times \prod_{a \in \mathcal{A}_P} \mathcal{E}_a. \tag{3.194}$$

We proceed exactly the same way for the remaining components in $\mathcal{A}_C$, $\mathcal{A}_S$, and $\mathcal{N}$. For each node $n \in \mathcal{N}$, we define spaces

$$e_n = H^1(I_t) =: \mathcal{E}_n, \tag{3.195a}$$
$$p_n \in H^1(I_t) =: \mathcal{P}_n, \tag{3.195b}$$

as well as the component and collective state spaces

$$\begin{aligned} \mathcal{Y}_n &= \mathcal{E}_n \times \mathcal{P}_n, \\ \mathcal{Y}_{\mathcal{N}} &= \prod_{n \in \mathcal{N}} \mathcal{Y}_n \cong \left(H^1(I_t)\right)^{2 \cdot |\mathcal{N}|} \end{aligned} \tag{3.196}$$

For consumers and producers, the entire state is defined by the fluxes, such that we define

$$q_{s:in} \in H^1(I_t) =: \mathcal{M}_s^{in} \tag{3.197a}$$
$$q_{s:out} \in H^1(I_t) =: \mathcal{M}_s^{out} \tag{3.197b}$$
$$Q_{s:in} \in H^1(I_t) =: \mathcal{Q}_s^{in} \tag{3.197c}$$
$$Q_{s:out} \in H^1(I_t) =: \mathcal{Q}_s^{out} \tag{3.197d}$$

and

$$\mathcal{Y}_{\mathcal{A}_C/\mathcal{A}_S} = \prod_{s \in \mathcal{A}_C/\mathcal{A}_S} \underbrace{\left(\mathcal{M}_s^{in} \times \mathcal{M}_s^{out} \times \mathcal{Q}_s^{in} \times \mathcal{Q}_s^{out}\right)}_{\mathcal{Y}_s} \cong \left(H^1(I_t)\right)^{4 \cdot |\mathcal{A}_C|/4 \cdot |\mathcal{A}_S|} \tag{3.198}$$

for $s \in \mathcal{A}_S \cup \mathcal{A}_C$.

3.39 Definition (Definition of the abstract state space $\mathcal{Y}$)

*We define the **state space** $\mathcal{Y}$ as the cartesian product*

$$\mathcal{Y} = \mathcal{Y}_{\mathcal{A}_P} \times \mathcal{Y}_{\mathcal{A}_C} \times \mathcal{Y}_{\mathcal{A}_S} \times \mathcal{Y}_{\mathcal{N}} \tag{3.199}$$

of the Hilbert spaces, which we introduced in (3.194) - (3.198). Given a representation

$$\mathcal{Y} = \prod_{i=1}^{N_{\mathcal{Y}}} \mathcal{Y}_i, \tag{3.200}$$

of $\mathcal{Y}$ as the product of $N_{\mathcal{Y}}$, we canonically define the scalar product

$$(\mathbf{y}, \mathbf{y}')_{\mathcal{Y}} = \sum_{i=1}^{N_{\mathcal{Y}}} (\mathbf{y}_i, \mathbf{y}_i')_{\mathcal{Y}_i}, \qquad \mathbf{y}, \mathbf{y}' \in \mathcal{Y} \tag{3.201}$$

and the induced norm

$$\|\mathbf{y}\|_{\mathcal{Y}} = \sqrt{(\mathbf{y}, \mathbf{y})_{\mathcal{Y}}} \tag{3.202}$$

on $\mathcal{Y}$. By construction, $(\mathcal{Y}, (\cdot, \cdot)_{\mathcal{Y}})$ is again a Hilbert space.

Remark 3.40: Abstract state trajectory

Using $\mathcal{Y}$ defined as above, we can introduce a family of Hilbert spaces

$$\mathcal{X}_i = \begin{cases} H^1(\Omega_a), \mathcal{Y}_i = \mathcal{E}_a \\ \mathbb{R}, \text{else} \end{cases} \tag{3.203}$$

and define $\mathcal{X} = \prod_i \mathcal{X}_i$, such that

$$\mathcal{Y} = H^1(I_t, \mathcal{X}, \mathcal{X}^\star) \tag{3.204}$$

is well defined in the sense of DEFINITION *3.35* . Analogously, we define the family of Hilbert spaces

$$\mathcal{X}_i^0 = \begin{cases} L^2(\Omega_a), \mathcal{Y}_i = \mathcal{E}_a \\ \mathbb{R}, \text{else} \end{cases} \tag{3.205}$$

and set $\mathcal{X}^0 = \prod_i \mathcal{X}_i$. By the construction above, we have that

$$\mathcal{X} \overset{compact}{\hookrightarrow} \mathcal{X}^0 \overset{continuous}{\hookrightarrow}, \mathcal{X}^\star \tag{3.206}$$

such $(\mathcal{X}, \mathcal{X}^0, \mathcal{X}^\star)$ is a Gelfand triple, and that the embeddings

$$\mathcal{Y} \hookrightarrow C^0\big(\bar{I}_t, \mathcal{X}^0\big), C^0\big(\bar{I}_t, \mathcal{X}^\star\big) \tag{3.207}$$

are continuous (i.e. $\mathbf{y} \in \mathcal{Y}$ has a time-continuous representative), and the embeddings

$$\mathcal{Y} \hookrightarrow L^2\big(I_t, \mathcal{X}^0\big), L^2(I_t, \mathcal{X}^\star) \tag{3.208}$$

are even compact. The last result is a consequence of the Aubin-Lions "lemma" THEOREM *3.41* . From this point of view, it is valid to define ***state trajectory*** $\{\mathbf{y}(t)\}_{t\in I_t}$ as a continuous curve with values in a infinite dimensional Hilbert space. The compact embedding ensures, that every bounded sequence in $\mathcal{Y}$ has a subsequence, which strongly converges in $L^2\big(I_t, \mathcal{X}^0\big)$ and $L^2(I_t, \mathcal{X}^\star)$.

3.41 Theorem (Aubin-Lions)

Let X_0, X_1, X_2 be Banach spaces, such that the embedding $X_0 \hookrightarrow X_1$ is compact, and $X_1 \hookrightarrow X_2$ is continuous. For $1 \leq p, q \leq \infty$, we define the space

$$W^{1,p,q} = \left\{ f \in L^p(I_t, X_0) \,\middle|\, \frac{d}{dt} f \in L^q(I_t, X_2) \right\} \tag{3.209}$$

of functions in $L^p(I_t, X_0)$, whose distributional derivative can be identified with a function in $L^q(I_t, X_2)$. Then the following holds true:

- *If $p < \infty$, the embedding $W \hookrightarrow L^p(I_t, X_1)$ is compact.*
- *If $p = \infty$ and $q > 1$, the embedding $W \hookrightarrow C^0\big(\bar{I}_t, X_1\big)$ is compact.*

Proof. [Aubin, 1963] □

For the construction of the control space we proceed in the same way:

3.42 Definition (Space of control variable $\mathcal{U}$)

*Let $s_0 \in \mathcal{A}_S$ denote the **primary source**. For each $s \in \mathcal{A}_S$, we define the space of its control variables as*

$$\mathcal{U}_s := \begin{cases} \mathcal{U}_s^e \times \mathcal{U}_s^{\Delta p} \times \mathcal{U}_s^{p_0}, & s = s_0 \\ \mathcal{U}_s^e \times \mathcal{U}_s^{\Delta p}, & \text{else} \end{cases} \tag{3.210}$$

*where we identify all space $\mathcal{U}_s^\bullet \cong H^1(I_t)$. We define the **space of control variables** $\mathcal{U} := \prod_{s\in\mathcal{A}_S} \mathcal{U}_s$.*
Further, let $u_s^{e,min}, u_s^{e,max}, u_s^{\Delta p,min}, u_s^{\Delta p,max}, u_{s_0}^{p_0,min}, u_{s_0}^{p_0,max} \in L^\infty(I_t)$, such that

$$\max_{c\in\mathcal{A}_C} e_c^{ret} < u_s^{e,min} < u_s^{e,max} \qquad \forall s \in \mathcal{A}_S, \tag{3.211a}$$

$$u_s^{\Delta p,min} < u_s^{\Delta p,max} \qquad \forall s \in \mathcal{A}_S, u_{s_0}^{p_0,min} < u_{s_0}^{p_0,max} \tag{3.211b}$$

and define the closed, convex subsets

$$\mathcal{U}_s^{e,ad} := \left\{ u_s^e \in \mathcal{U}_s^e \,\middle|\, u_s^{e,min} \le u_s^e \le u_s^{e,max} \right\} \tag{3.212a}$$

$$\mathcal{U}_s^{\Delta p,ad} := \left\{ u_s^{\Delta p} \in \mathcal{U}_s^{\Delta p} \,\middle|\, u_s^{\Delta p,min} \le u_s^{\Delta p} \le u_s^{\Delta p,max} \right\} \tag{3.212b}$$

$$\mathcal{U}_{s_0}^{p_0,ad} := \left\{ u_{s_0}^{p_0} \in \mathcal{U}_{s_0}^{p_0} \,\middle|\, u_{s_0}^{p_0,min} \le u_{s_0}^{p_0} \le u_{s_0}^{p_0,max} \right\} \tag{3.212c}$$

*of $\mathcal{U}_s^e$, $\mathcal{U}_s^{\Delta p}$, and $\mathcal{U}_{s_0}^{p_0}$. We define the **set of feasible controls** as $\mathcal{U}^{ad} := \prod_{s\in\mathcal{A}_S} \mathcal{U}_s^{ad}$.*

Next, we are going to construct the residual

$$\mathcal{G} : \mathcal{U} \times \mathcal{Y} \to \mathcal{Z}^\star \tag{3.213}$$

as a Cartesian product operators as formal residuals of state equations. For now, we are going to assume that $\mathcal{Z}$ (and its dual $\mathcal{Z}^\star$) is given as the Cartesian product of finitely many Banach spaces, whose precise definition is going to be given in DEFINITION *3.43* at the end of this section.
From SECTION *3.2.2* we already know that the mapping

$$(v_a, e_a) \longmapsto \begin{pmatrix} \displaystyle\int_{I_t} \left\langle \frac{d}{dt} e_a, z_a^{adv} \right\rangle_{H^1(\Omega_a)^\star, H^1(\Omega_a)} dt \\ z_a^{adv} \mapsto + \displaystyle\int_{I_t} \left(v_a(t) \partial_x e_a(t), z_a^{adv} \right)_{L^2(\Omega_a)} dt \\ + \displaystyle\int_{I_t} \left(r\left(e_a(t)\right), z_a^{adv} \right)_{L^2(\Omega_a)} dt \end{pmatrix} \tag{3.214}$$

is well-defined for every *test function* $z_a^{adv} \in L^2\big(I_t, H^1(\Omega_a)\big)$. Therefore, it naturally extends to a mapping

$$\mathcal{G}_a^{adv} : \mathcal{V}_a \times \mathcal{E}_a \longrightarrow \mathcal{E}_a^\star =: \left(\mathcal{Z}_a^{adv}\right)^\star \tag{3.215}$$

We define the residual operator $\mathcal{G}_a^{adv}$ of the advection equation for each pipe $a \in \mathcal{A}_P$ as

$$\begin{aligned}\left\langle \mathcal{G}_a^{adv}(\mathbf{u},\mathbf{y}),\mathbf{z}\right\rangle_{\mathcal{E}_a^\star,\mathcal{E}_a} \coloneqq &\int_{I_t}\left\langle \frac{d}{dt}e_a(t), z_a^{adv}(t)\right\rangle_{H^1(\Omega_a)^\star,H^1(\Omega_a)} dt\\ &+\int_{I_t}\left(v_a(t)\partial_x e_a(t), z_a^{adv}(t)\right)_{L^2(\Omega_a)} dt\\ &+\int_{I_t}\left(r\left(e_a\right)(t), z_a^{adv}(t)\right)_{L^2(\Omega_a)} dt.\end{aligned} \tag{3.216}$$

From LEMMA 3.37 and the discussion preceding it, we already know that the expression

$$\mathcal{G}_a^{e:in}(\mathbf{u},\mathbf{y}) = e_{a:in} - e_{i(a)} \tag{3.217}$$

needs some clarification, if e_a is an arbitrary element of $\mathcal{E}_a$. In general, we cannot expect $tr_0 : \mathcal{E}_a \to H^1(I_t)$ to hold, as we can only rely on the significantly weaker property $tr_0 : \mathcal{E}_a \to L^2(I_t)$.
For each edge $a \in \mathcal{A}$ and $n \in \{i(a), o(a)\}$, we define the symbol

$$e_{a:n} = \begin{cases} e_{i(a)}, & a \in \mathcal{A}\setminus\mathcal{A}_P, n = i(a)\\ e_{o(a)}, & a \in \mathcal{A}\setminus\mathcal{A}_P, n = o(a)\\ tr_0 e_a, & a \in \mathcal{A}_P, n = i(a)\\ tr_{L_a} e_a, & a \in \mathcal{A}_P, n = o(a)\end{cases} \tag{3.218}$$

such that we can maintain the uniform notation introduced in CHAPTER 2.
Technically, we could formulate the inflow boundary conditions in terms of a L^2 identity. In order to preserve the structure given by the weak formulation $\mathcal{G}^{adv}$ of the advection operator, we use the Gelfand triple structure of $\left(H^1, L^2, H^{1\star}\right)$ and obtain the weak formulation

$$\left\langle \mathcal{G}_a^{e:in}(\mathbf{u},\mathbf{y}),\mathbf{z}\right\rangle_{H^1(I_t)^\star,H^1(I_t)} \coloneqq \int_{I_t}\left(e_{a:in}(t) - e_{i(a)}(t)\right)\cdot z_a^{e:in}(t)\, dt. \tag{3.219}$$

of the inflow boundary conditions.
We note, that if e_a solves the equation $\mathcal{G}_a^{e:in}(\mathbf{u},\mathbf{y}) = 0$ in $H^1(I_t)^\star$, we get that

$$\left\|\mathcal{G}_a^{e:in}(\mathbf{u},\mathbf{y})\right\|_{H^1(I_t)^\star} = \sup_{\|z_a^{e:in}\|_{H^1(I_t)}\le 1}\left|\int_{I_t}\left(e_{a:in}(t) - e_{i(a)}(t)\right)\cdot z_a^{e:in}(t)\, dt\right| = 0 \tag{3.220}$$

and $e_{a:in} = e_{i(a)}$ almost everywhere in I_t. If $e_{i(a)}$ is a function in $H^1(I_t)$, we immediately conclude that $e_{a:in} = tr_0 e_a =\in H^1(I_t)$. This justifies to use the formal notation (3.217), if we keep in mind that its actual meaning is given by (3.219).
By THEOREM 3.36 we can apply the same reasoning for the initial conditions of the advection problem, and write

$$\mathcal{G}_a^{init} = e_a(t_0) - e_a^{init} \tag{3.221}$$

where the actual meaning of this expression is given by the dual pairing

$$\left\langle \mathcal{G}_a^{init}(\mathbf{u},\mathbf{y}),\mathbf{z}\right\rangle_{H^1(\Omega_a)^\star,H^1(\Omega_a)} \coloneqq \int_{\Omega_a} z_a^{init}(x)\left(e_a(t_0)(x) - e_a^{init}(x)\right)\, dx. \tag{3.222}$$

Following this procedure, the weak formulation of the hydraulic equation is given by

$$\begin{aligned}\left\langle \mathcal{G}_a^{hyd}(\mathbf{u},\mathbf{y}),\mathbf{z}\right\rangle_{H^1(I_t)^\star,H^1(I_t)} = &\int_{I_t} z_a^{hyd}(t)\left(p_{o(a)}(t) - p_{i(a)}(t)\right)\, dt\\ &+\int_{I_t} z_a^{hyd}(t)\left(g\frac{\Delta h_a}{L_a} + \frac{\lambda_a}{2d_a}v_a\left|v_a\right|(t)\right)\int_{\Omega_a}\rho\left(e_a\right)(t)(x)\, dx\, dt\end{aligned} \tag{3.223}$$

such that $\mathcal{G}_a^{hyd}$ should define a mapping

$$\mathcal{G}_a^{hyd} : \mathcal{V}_a \times \mathcal{E}_a \times \mathcal{P}_{i(a)} \times \mathcal{P}_{o(a)} \longrightarrow H^1(I_t)^\star =: \left(\mathcal{Z}_a^{hyd}\right)^\star . \tag{3.224}$$

So far, the assumptions regarding ρ have been rather general. Since we cannot guarantee, that a continuous representative of e_a exists, we will have to require additional properties for ρ in order for $\mathcal{G}_a^{hyd}$ to form a well defined mapping in the sense of (3.224).

We briefly summarize all coupling equations of the system, starting with the initial and boundary conditions

$$\mathcal{G}_a^{e:init}(\mathbf{u},\mathbf{y}) = e_a(t_0) - e_a^{init}, \tag{3.225}$$

$$\mathcal{G}_a^{e:in}(\mathbf{u},\mathbf{y}) = e_{a:in} - e_{i(a)}, \tag{3.226}$$

for each pipeline $a \in \mathcal{A}_P$, and the mass and energy fluxes

$$\mathcal{G}_a^{q:in}(\mathbf{u},\mathbf{y}) = q_{a:in} + v_a A_a, \tag{3.227a}$$

$$\mathcal{G}_a^{q:out}(\mathbf{u},\mathbf{y}) = q_{a:in} - v_a A_a, \tag{3.227b}$$

$$\mathcal{G}_a^{Q:in}(\mathbf{u},\mathbf{y}) = Q_{a:in} - q_{a:in} e_{a:in}, \tag{3.228a}$$

$$\mathcal{G}_a^{Q:out}(\mathbf{u},\mathbf{y}) = Q_{a:out} - q_{a:out} e_{a:out}. \tag{3.228b}$$

We highlight, that $\mathcal{G}^{q:in}$, and $\mathcal{G}^{q:out}$ can be interpreted safely as mappings with values in $H^1(I_t)$, whereas $\mathcal{G}^{Q:in}$, and $\mathcal{G}^{q:out}$ explicitly depend on the trace of e_a. The fluxes and algebraic coupling conditions of consumers $c \in \mathcal{A}_C$

$$\mathcal{G}_c^{Q:in}(\mathbf{u},\mathbf{y}) = Q_{c:in} - q_{c:in}\phi_c\left(e_{i(c)}\right), \tag{3.229a}$$

$$\mathcal{G}_c^{Q:out}(\mathbf{u},\mathbf{y}) = Q_{c:out} - q_{c:out} e_c^{ret}, \tag{3.229b}$$

$$\mathcal{G}_c^{\Delta\hat{q}}(\mathbf{u},\mathbf{y}) = \rho\left(\phi_c(e_{i(c)})\right) q_{c:in} + \rho\left(e_c^{ret}\right) q_{c:out}, \tag{3.230a}$$

$$\mathcal{G}_c^{\Delta Q}(\mathbf{u},\mathbf{y}) = Q_{c:in} + Q_{c:out} + Q_c^{pred}, \tag{3.230b}$$

and the producer

$$\mathcal{G}_s^{Q:in}(\mathbf{u},\mathbf{y}) = Q_{s:in} - q_{s:in} e_{i(s)}, \tag{3.231a}$$

$$\mathcal{G}_s^{Q:out}(\mathbf{u},\mathbf{y}) = Q_{s:out} - q_{s:out} u^e, \tag{3.231b}$$

$$\mathcal{G}_s^{p0}(\mathbf{u},\mathbf{y}) = p_{i(s)} - u_s^{p_0}, \tag{3.232a}$$

$$\mathcal{G}_s^{\Delta p}(\mathbf{u},\mathbf{y}) = p_{o(s)} - p_{i(s)} - u_s^{\Delta p}, \tag{3.232b}$$

are less problematic, because all state variables involved are elements of $H^1(I_t)$, and we can rely on their respective continuous representative. are interpreted as mapping with values in $H^1(I_t)$. Like in the case of $\mathcal{G}^{hyd}$, we call attention to the detail, that some of these operators depend on the composition of the functions ρ and ϕ_c.

Finally, we conclude the formal construction of the weak residual formulation with the nodal conservation laws for mass and energy

$$\begin{aligned}\left\langle \mathcal{G}_n^{\Delta\hat{q}}(\mathbf{u},\mathbf{y}), z_n^{\Delta\hat{q}} \right\rangle_{H^1(I_t)^\star, H^1(I_t)} &:= \int_{I_t} z_n^{\Delta\hat{q}}(t) \left(\sum_{a \in I(n)} q_{a:n}(t) \rho\left(e_{a:n}\right)(t) \right) dt \\ &= \sum_{a \in I(n)} \left(\int_{I_t} z_n^{\Delta\hat{q}}(t) q_{a:n}(t) \rho\left(e_{a:n}\right)(t)\, dt \right)\end{aligned} , \tag{3.233a}$$

$$\left\langle \mathcal{G}_n^{\Delta Q}(\mathbf{u},\mathbf{y}), z_n^{\Delta Q} \right\rangle_{H^1(I_t)^\star, H^1(I_t)} := \int_{I_t} z_n^{\Delta Q}(t) \left(\sum_{a \in I(n)} Q_{a:n}(t) \right) dt \quad . \tag{3.233b}$$

Again, we emphasize that these formally defined operators involve the superposition of the function ρ with the trace operator, as well as multilinear products. We summarize these results in the following definition:

3.43 Definition (Residual operator $\mathcal{G}$ and weak solutions)

Let $(\mathcal{N}, \mathcal{A})$ be the graph representation of a simple district heating network in the sense of DEFINITION 2.6*. Further, let $\mathcal{Y}$ be the Hilbert spaces given in* DEFINITION 3.39*, $\mathcal{Y}$ the space of controls, and $\mathcal{Y}^{ad}$ a closed, convex feasible subset according to* DEFINITION 3.42*.*
Analogously to the construction of $\mathcal{Y}$, we construct the function spaces

$$\mathcal{Z}_a = \mathcal{E}_a \times \mathcal{V}_a \times H^1(\Omega_a) \times \left(H^1(I_t)\right)^5 \tag{3.234a}$$
$$\mathcal{Z}_c = \left(H^1(I_t)\right)^4 \tag{3.234b}$$
$$\mathcal{Z}_s = \left(H^1(I_t)\right)^4 \tag{3.234c}$$
$$\mathcal{Z}_n = \left(H^1(I_t)\right)^2 \tag{3.234d}$$

as for each $a \in \mathcal{A}_P$, $c \in \mathcal{A}_C$, $n \in \mathcal{N}$, and the single producer s.
*We define the **space of test functions** (or **adjoint state space**) $\mathcal{Z}$ as*

$$\mathcal{Z} = \left(\prod_{a\in\mathcal{A}_P} \mathcal{Z}_a\right) \times \left(\prod_{c\in\mathcal{A}_C} \mathcal{Z}_c\right) \times \left(\prod_{n\in\mathcal{N}} \mathcal{Z}_n\right) \times \mathcal{Z}_s \tag{3.235}$$

which is the finite Cartesian product of Hilbert spaces, and therefore a Hilbert space.
In the same way we define the operators

$$\mathcal{G}_{a,c,s,n} : \mathcal{U} \times \mathcal{Y} \to \mathcal{Z}^\star_{a,c,s,n} \tag{3.236}$$

in terms of (3.216)-(3.233)*, such that their Cartesian product*

$$\mathcal{G} = \left(\prod_{a\in\mathcal{A}_P} \mathcal{G}_a\right) \times \left(\prod_{c\in\mathcal{A}_C} \mathcal{G}_c\right) \times \left(\prod_{n\in\mathcal{N}} \mathcal{G}_n\right) \times \mathcal{G}_s \tag{3.237}$$

formally defines an operator

$$\mathcal{G} : \mathcal{U} \times \mathcal{Y} \to \mathcal{Z}^\star \tag{3.238}$$

*whose image lies in the space of continuous, linear functionals on $\mathcal{Z}$. Given $\mathbf{u} \in \mathcal{U}^{ad}$, we say that $\mathbf{y}$ is a **weak solution** of* (2.94)-(2.103)*, if $\mathcal{G}(\mathbf{y}, \mathbf{u})$ is defined and bounded for $\mathbf{y}$, and*

$$\langle \mathcal{G}(\mathbf{u}, \mathbf{y}), \mathbf{z} \rangle_{\mathcal{Z}^\star, \mathcal{Z}} = 0 \tag{3.239}$$

holds for all test vectors $\mathbf{z} \in \mathcal{Z}$. Equivalently one could say, that $\mathcal{G}(\mathbf{u}, \mathbf{y}) = 0_{\mathcal{Z}^\star}$ is a functional, which identically vanishes for all $\mathbf{z} \in \mathcal{Z}$.

The operator $\mathcal{G}$ given in the definition above is only formally defined, since it is not necessarily bounded. This is intended, since we want to defer the discussion regarding the superposition operators ρ and ϕ_c to SECTION 3.3.2 and SECTION 3.3.3, where we deal with the continuity and differentiability of $\mathcal{G}$.

In order to simplify the further analysis of $\mathcal{G}$, we note that the construction of $\mathcal{Y}$, $\mathcal{U}$, $\mathcal{Z}$, and

$\mathcal{G}$ as finite Cartesian products allows for a decomposition of the weak formulation

$$\begin{aligned}\langle \mathcal{G}(\mathbf{u},\mathbf{y}),\mathbf{z}\rangle_{\mathcal{Z}^\star,\mathcal{Z}} = &\sum_{a\in\mathcal{A}_P}\langle \mathcal{G}_a(\mathbf{u},\mathbf{y}),\psi_a\mathbf{z}_a\rangle_{\mathcal{Z}_a^\star,\mathcal{Z}_a} + \sum_{c\in\mathcal{A}_C}\langle \mathcal{G}_c(\mathbf{u},\mathbf{y}),\psi_c\mathbf{z}_c\rangle_{\mathcal{Z}_c^\star,\mathcal{Z}_c}\\ &+\sum_{n\in\mathcal{N}}\langle \mathcal{G}_n(\mathbf{u},\mathbf{y}),\psi_n\mathbf{z}_n\rangle_{\mathcal{Z}_n^\star,\mathcal{Z}_n} + \langle \mathcal{G}_s(\mathbf{u},\mathbf{y}),\psi_s\mathbf{z}_s\rangle_{\mathcal{Z}_s^\star,\mathcal{Z}_s},\end{aligned} \tag{3.240}$$

into finite sums, where

$$\psi_i : \mathcal{Z}_i \to \mathcal{Z} \tag{3.241}$$

are the canonical embeddings of $\mathcal{Z}_{a,c,s,n}$ into $\mathcal{Z}$. In particular, one can rearrange each individual term without changing the equation, and study not only component wise, but also term wise.

3.3.2 Weak continuity and boundedness of $\mathcal{G}$

In a first step, we are going to analyse the continuity and boundedness properties of $\mathcal{G}$. As we have already seen in the preceding section, most terms of $\mathcal{G}$ are bounded by construction, and the only critical parts are those ones, which are generated by superposition with a (possibly non-linear) function.
As pointed out in the introduction, one of our main goals is to establish a toolset for handling optimal control problems for district heating networks. In CHAPTER 4 we are going to prove the existence of local minima of certain optimization problems involving $\mathcal{G}$ by minimizing sequences. Due to the lack of compactness, the boundedness of $\mathcal{G}$ and the cost functional are only enough to deduce the existence of a *weakly convergent* minimizing sequence, whereas strong convergence cannot be proven in the general case.
If the system's dynamics were to be modelled by a continuous, linear operator L with continuous, linear adjoint $L^\star$, we have

$$\langle Lx_n, z\rangle = \langle x_n, L^\star z\rangle \to \langle x, L^\star z\rangle \tag{3.242}$$

such that the Lx_n converges weakly in $\mathcal{Z}^\star$. In general, this is does not hold in the non-linear case.

3.44 Definition (Weak-weak* continuity of operators)

*Let $(X,\|\cdot\|_X),(Y,\|\cdot\|_Y)$, be reflexive Banach spaces. A (possibly non-linear) operator $N : X \to Y^\star$ is called **weak-weak*-continuous**, if for every sequence $(x_n)_n \subset X$, which weakly converges in X, the sequence $N(x_n)$ converges weakly in $Y^\star$, i.e.*

$$\langle f, x_n\rangle_{X^\star,X} \to \langle f,x\rangle_{X^\star,X}\ \forall f\in X^\star \Rightarrow \langle N(x_n),y\rangle_{Y^\star,Y} \to \langle N(x),y\rangle_{X^\star,X}\ \forall y\in Y. \tag{3.243}$$

In our case, most non-linearities are either generated by a superposition

$$u \mapsto \left(z \mapsto \int_{I_t} \phi(u)(t)\cdot z(t)\,dt\right) \tag{3.244}$$

of a function in $H^1(I_t)$ with a (possibly non-linear) function ϕ, or multilinear expressions of the form

$$(u,v) \mapsto \left(z \mapsto \int_{I_t} v(t)\cdot\langle F(u)(t), z(t)\rangle_{H^1(\Omega)^\star,H^1(\Omega)}\,dt\right), \tag{3.245}$$

where $F : H^1\big(I_t, H^1(\Omega), H^1(\Omega)^\star\big) \to H^1(I_t)^\star$ is assumed to be at least continuous.
Both cases are examples of *Nemitskii operators* between (subspaces of) Banach spaces of the form $L^p(I_t, X)$, and $L^q(I_t, Y)$.
The requirements on F and ϕ, such that the resulting Nemitskii operators are (weakly) continuous, or even differentiable, are quite strong (especially in the case $p = q$). For a broader discussion of this topic we refer to [Goldberg et al., 1992].
Here we can already observe, that weak-weak* is strictly stronger than strong continuity, since that the last limit cannot hold, if *both* sequences only weakly converge in $L^2(I_t)$.

Remark 3.45: Extension of Lipschitz function to all of $\mathbb{R}$

The superposition operators, which cause most of the non-linearities in our model equations, all originate from (bounded) Lipschitz functions, which have only been defined on a (compact) subset of $\mathbb{R}$. This was sufficient for the study of existence and uniqueness of solutions in SECTION 3.1 and SECTION 3.2 . In the case of the weak residual formulation, in particular in the context of optimal control, we want $\mathcal{G}$ to be well defined even outside the solution space.
We briefly outline a construction, which extends such functions the whole real line, and thereby maintains boundedness, Lipschitz continuity, and (if needed) differentiability.
Let $[a, b] \subset \mathbb{R}$ be a non-empty real interval, and $f \in C^1([a, b])$, with upper and lower bounds $f^{min} \leq f \leq f^{max}$. We define the extension of f as a piecewise function

$$\tilde{f}(x) = \begin{cases} f_p(\tilde{a}), & x < \tilde{a} \\ f_p(x), & \tilde{a} \leq x \leq a \\ f(x), & a < x < b \\ f_q(x), & b \leq x \leq \tilde{b} \\ f_q(\tilde{b}), & x > \tilde{b} \end{cases} \tag{3.246}$$

where the transition functions f_p and f_q are constructed as cubic Bézier curves with control polygons $p^i \in \mathbb{R}^2, i = 0, \dots, 3$, and $q^i \in \mathbb{R}^2, i = 0, \dots, 3$. For the entire set of conditions for continuity and higher order coupling conditions we refer to [Quarteroni et al., 2007]. We want to highlight a special case for the C^1 continuity condition

$$p_y^2 = f(a) - f'(a)\left(a - p_x^2\right) \tag{3.247}$$

at the left boundary of the interval. In the case, that $f'(a) > 0$ and $f(a) = f^{min}$ (analogously $f'(a) < 0$ and $f(a) = f^{max}$), we cannot define $\tilde{f}$ in such a way, that the original bounds still hold.
However, given any constant $\delta \geq 0$, we can construct the Bézier curve in such a way, that

$$f^{min} - \delta < \tilde{f}^{min} \leq \tilde{f} \leq \tilde{f}^{max} < f^{max} + \delta \tag{3.248}$$

always holds true. The additional parameter δ gives some flexibility for practical applications, but is not as relevant for theoretical investigations. Obviously, there exist many other ways to perform such a construction, and this one merely serves as an explicit example.

We begin with the simplest case, which only involves the superposition of a single Sobolev function with a Lipschitz function.

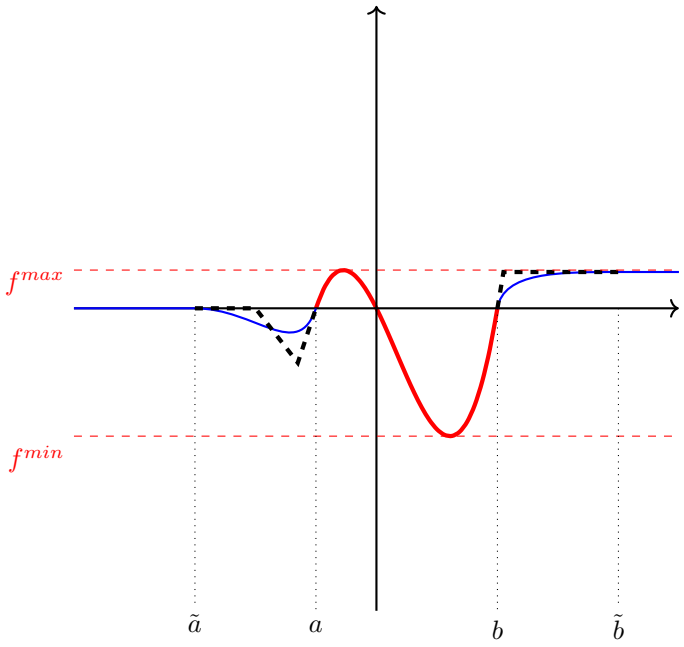

Figure 3.4: Illustration of the extension procedure, which is outlined in REMARK 3.45

3.46 Lemma (Boundedness and weak-weak* continuity of Nemitskii operators I)

Let $\phi : \mathbb{R} \to \mathbb{R}$ be a globally Lipschitz continuous function. Then the superposition mapping $y \mapsto \phi(y)$ induces a bounded operator

$$N_\phi : H^1(I_t) \to H^1(I_t)^\star$$
$$\langle N_\phi(y), z \rangle_{H^1(I_t)^\star, H^1(I_t)} := \int_I \phi(y)(t) z(t)\, dt, \tag{3.249}$$

which is bounded and weak-weak* continuous.

Proof. Because the function ϕ is globally Lipschitz by assumption, it is bounded on bounded intervals, and the operator N_ϕ is bounded in L^2. The derivative of ϕ exists almost everywhere, such that the weak derivative of $\phi(y)$ is well defined for every $y \in H^1(I_t)$ by LEMMA 3.16. In particular, N_ϕ is bounded in $H^1(I_t)$.

For the second statement, let y_n be a weakly convergent sequence in $H^1(I_t)$. We are going to prove that $\phi(y_n)$ converges weakly in $H^1(I_t)$. From the compact embedding $H^1(I_t) \mapsto L^2(I_t)$ (see LEMMA 3.14), we conclude the existence of a subsequence, which strongly converges in $L^2(I_t)$. In the following we are going to select an arbitrary, strongly convergent subsequence, which we again refer to as y_n. Because ϕ is Lipschitz continuous, the sequence $\eta_n := \phi(y_n)$ is bounded in H^1 (this follows from LEMMA 3.16, and the embedding into L^2). We can conclude, that there exists a subsequence (which we also refer to as η_n), such that $\eta_n \rightharpoonup \eta$ in $H^1(I_t)$. Again, we utilize the compact embedding into L^2 to see, that $\eta_n \to \tilde{\eta}$ in L^2.

Together with the continuity of ϕ, we finally obtain $\eta_n = \phi(y_n) \rightharpoonup \phi(y) = \eta \in H^1(I_t)$.

Now, let $z \in H^1(I_t)$ be arbitrary but fixed. Using the definition of N_ϕ in (3.249), we can see

that

$$y \mapsto \int_I \phi(y)(t)z(t)\,dt \tag{3.250}$$

is a continuous, linear functional on $H^1(I_t)$. Therefore, we can establish the limit

$$\langle N_\phi(y_n), z\rangle_{H^1(I_t)^\star, H^1(I_t)} \to \langle N_\phi(y), z\rangle_{H^1(I_t)^\star, H^1(I_t)}\,, \tag{3.251}$$

since $\phi(y_n)$ converges weakly, and N_ϕ is weak-weak*-continuous. □

This result can be immediately generalized to multivariate operators, since the product of finitely many Lipschitz functions is again Lipschitz.

3.47 Lemma (Boundedness and weak-weak* continuity of Nemitskii operators II)

Let $\mathcal{K}$ be a finite index set, and $y_k \in H^1(I_t) \forall k \in \mathcal{K}$. Further, let $f_k : \mathbb{R} \to \mathbb{R}$ be family globally Lipschitz continuous functions. Then the function

$$F(y)(t) = \prod_{k\in\mathcal{K}} f_k\left(y_k\right)(t) \tag{3.252}$$

is an element of $H^1(I_t)$, and the operator $N_F : \prod_{k\in\mathcal{K}} H^1(I_t) \to H^1(I_t)^\star$, defined by

$$\langle N_F(y), z\rangle_{H^1(I_t)^\star, H^1(I_t)} = \int_{I_t} F(y)(t)z(t)\,dt \tag{3.253}$$

is bounded and weak-weak*-continuous.

Proof. The space $H^1(I_t)$ is closed under (pointwise) multiplication, and composition with Lipschitz functions. Since F is constructed as the finite product of Lipschitz function, it is Lipschitz continuous w.r.t. its arguments y_k, and therefore $F \in H^1(I_t)$.
By LEMMA 3.14, every y_k has a unique $C^0(\bar{I}_t)$ representative, such that we can derive explicit bounds $f_k^{max} = \|f_k\|_{C^0([-y_k^{max}, y_k^{max}])}$ for each f_k, where $y_k^{max} = \|y_k\|_\infty$. By using these explicit bounds, we can immediately see that

$$\left|\langle N_F(y), z\rangle_{H^1(I_t)^\star, H^1(I_t)}\right| \leq \underbrace{\left(\prod_{k\in\mathcal{K}} f_k^{max}\right)}_{F^{max}} \|z\|^2_{H^1(I_t)} \tag{3.254}$$

holds for all $z \in H^1(I_t)$, such that N_F is bounded. The weak-weak*-continuity follows analogously to the proof of LEMMA 3.46. □

As we have seen in LEMMA 3.37, and LEMMA 3.38 the trace operator on $L^2\left(I_t, H^1(\Omega)\right)$ is a L^2 valued, linear, and weak-weak*-continuous operator. When we consider the superposition of the trace with another function, we generally have to restrict ourselves to the affine and linear ones (see [Goldberg et al., 1992]).

3.48 Definition (Affine operator)

Let $(X, \|\cdot\|_X)$, $(Y, \|\cdot\|_Y)$ be Banach spaces. An operator

$$A : X \to Y \tag{3.255}$$

*is called **affine**, if there exists a unique $y_0 \in Y$, and a linear operator $L : X \mapsto Y$, such*

that

$$A(x) = Lx + y_0. \tag{3.256}$$

An affine operator is called continuous, if and only if L is continuous.

If X and Y are real function spaces it is easy to see, that the superposition with an affine function $a(x) = a_0 + a_1 x$ yields a bounded, affine operator, if and only if constant functions are bounded in Y. This leads to the following statement:

3.49 Lemma (Boundedness and weak-weak* continuity of Nemitskii operators III)

Let $(X, \|\cdot\|_X)$ be a Banach space, and $A : X \to L^2(I_t)$ a continuous, affine operator. We define the operator $B : X \times H^1(I_t) \to H^1(I_t)^\star$ by

$$\langle B(x,y), \omega \rangle_{H^1(I_t)^\star, H^1(I_t)} = \int_{I_t} (Ax)(t) y(t) \omega(t)\, dt \tag{3.257}$$

for every $z \in H^1(I_t)$. Then B is bounded, and weak-weak* continuous.

Proof. We split the affine operator into its linear part $L = A - a_0$, and the constant remainder term $a_0 \in L^2(I_t)$. Since $H^1(I_t)$ is compactly embedded into $L^2(I_t)$, the *remainder* operator

$$\langle R(y), z \rangle_{H^1(I_t)^\star, H^1(I_t)} \int_{I_t} a_0(t) \cdot y(t) \cdot z(t)\, dt \tag{3.258}$$

is compact, and therefore bounded and weak-weak*-continuous.
Therefore, it is sufficient to only treat the special case $A \equiv L$, such that B is a bilinear operator.
Let $(w_n)_n, w_n = (x_n, y_n)$ be a weakly convergent sequence in $X \times L^2(I_t)$, and $\omega \in H^1(I_t)$ arbitrary but fixed. We make use of the subdivision

$$B(x_n, y_n) - B(x, y) = B(x_n - x, y) - B(x_n, y - y_n) \tag{3.259}$$

of B, such that we can examine both parts separately. The first part defines a continuous, linear functional

$$\langle f_y, x \rangle_{X^\star, X} \coloneqq \langle B(x_n - x, y), \omega \rangle_{H^1(I_t)^\star, H^1(I_t)} = \int_{I_t} (L(x_n - x))(t) y(t) \omega(t)\, dt \tag{3.260}$$

and therefore vanishes in the limit, since x_n converges weakly in X.
If we make use of the compact embedding $H^1(I_t) \hookrightarrow L^2(I_t)$, we conclude that y_n converges strongly in $L^2(I_t)$, and we obtain the norm estimate

$$\lim_{n\to\infty} \|y_n - y\|_{L^2(I_t)} = 0. \tag{3.261}$$

Because $\left(H^1(I_t), +, \cdot\right)$ is a function ring, the elements $z_n = y_n \omega$ also define a sequence in H^1. If we apply the Riesz representation theorem

$$\langle \varphi^\star, z_n \rangle_{H^1(I_t)^\star, H^1(I_t)} = (\varphi, y_n \omega)_{H^1(I_t)} = (\omega\varphi, y_n)_{H^1(I_t)}, \tag{3.262}$$

we can see, that the weak convergence of y_n carries over to z_n, such that $y_n \omega = z_n \rightharpoonup z = y\omega$, and

$$\lim_{n\to\infty} \|z_n - z\|_{L^2(I_t)} = \lim_{n\to\infty} \|(y_n - y)\omega\|_{L^2(I_t)} = 0. \tag{3.263}$$

Next, we observe that every weakly convergent sequence must be bounded, such that there exist a positive constant C_x satisfying $C_x \leq \|x_n\|_X$ for all n. This leads to the following estimate

$$\sup_{\omega \in H^1(I_t)} \left| \int_{I_t} (Lx_n)(t) y(y_n(t) - y(t)) \omega(t)\, dt \right| \leq C_x \|L\| \, \|(y_n - y)\omega\|_{L^2(I_t)} \tag{3.264}$$

where $\|L\|$ denotes the operator norm of the linear operator L.
This leads to the final estimate of the limit

$$\lim_{n\to\infty} \left| \int_{I_t} (Lx_n)(t) y(y_n(t) - y(t)) \omega(t)\, dt \right| \leq C_x \|L\| \lim_{n\to\infty} \|(y_n - y)\omega\|_{L^2(I_t)} = 0, \tag{3.265}$$

such that B is weak-weak*-continuous. □

Finally, we cover those bilinear operators, which involve integrals over a spatial Ω_a, namely $\mathcal{G}^{hyd}$ and $\mathcal{G}^{adv}$.

3.50 Lemma (Boundedness and weak-weak* continuity of Nemitskii operators IV)

Let $(X, \|\cdot\|_X)$ be a real Banach space, $Y = H^1(I_t)$, and $A : X \to L^2\big(I_t, H^1(\Omega)^\star\big) =: Z^\star$ a continuous, affine operator, and $\phi : \mathbb{R} \to \mathbb{R}$ a globally Lipschitz continuous function. Then the operator

$$\langle B(x,y), z\rangle_{Z^\star,Z} := \int_{I_t} \phi(y)(t) \cdot \langle A(x)(t), z(t)\rangle_{H^1(\Omega)^\star, H^1(\Omega)}\, dt, \tag{3.266}$$

is bounded, and weak-weak* continuous.

Proof. Let x_n, y_n be weakly convergent sequences. We start with the simplified case, where ϕ is the identity function. As in the proof of LEMMA 3.49, we split A into its linear part L, and constant remainder a_0. We see that the remainder term is bounded by

$$\left| \int_{I_t} y(t) \cdot \langle a_0(t), z(t)\rangle_{H^1(\Omega)^\star, H^1(\Omega)}\, dt \right| \leq \|y\|_\infty \int_{I_t} \left| \langle a_0(t), z(t)\rangle_{H^1(\Omega)^\star, H^1(\Omega)} \right| dt < \infty. \tag{3.267}$$

Now we use $f(t) = \langle a_0(t), z(t)\rangle_{H^1(\Omega)^\star, H^1(\Omega)} \in L^2(I_t)$ and apply our standard compact embedding argument on $H^1(I_t)$ to see that it is weak-weak*-continuos w.r.t. y.
For the linear part, boundedness follows in the same way, and we have

$$\left| \int_{I_t} y(t) \cdot \langle Lx(t), z(t)\rangle_{H^1(\Omega)^\star, H^1(\Omega)}\, dt \right| \leq \|y\|_\infty \int_{I_t} \left| \langle Lx(t), z(t)\rangle_{H^1(\Omega)^\star, H^1(\Omega)} \right| dt < \infty, \tag{3.268}$$

since L is assumed to be bounded.
Like in the proof of LEMMA 3.49, we now consider the special case $a_0 \equiv 0$, such that B is assumed to be bi-linear, and we can perform the splitting

$$B(x_n, y_n) - B(x, y) = B(x_n - x, y) - B(x_n, y - y_n). \tag{3.269}$$

For the second term, we combine the standard compactness argument for y_n, and use that

$$\langle Lx_n(t), z(t)\rangle_{H^1(\Omega)^\star, H^1(\Omega)} \to \langle Lx(t), z(t)\rangle_{H^1(\Omega)^\star, H^1(\Omega)} \tag{3.270}$$

for almost every $t \in I_t$, from which we conclude the boundedness and weak-weak*-continuity by the same argument as in LEMMA 3.49.
For the first term, we rewrite the inner dual pairing

$$\langle L(x_n - x)(t), z(t)\rangle_{H^1(\Omega)^\star, H^1(\Omega)} = \langle (x_n - x)(t), L^\star z(t)\rangle_{X, X^\star} \tag{3.271}$$

in terms of the adjoint of the linear part of A, such that we obtain a linear functional $L^\star z \in X^\star$ for every $z \in Z$ at every time $t \in I_t$. In particular, the resulting function is an element of L^2 and

$$\langle x_n, L^\star z\rangle_{X, X^\star} \rightharpoonup \langle x, L^\star z\rangle_{X, X^\star} \quad \text{in } L^2(I_t), \tag{3.272}$$

such that the whole term is weak-weak*-continuous.
For the general case, we recall that in the proof LEMMA 3.46 we have shown, that the composition $\phi(y_n)$ also converges weakly in H^1. Therefore, the argument above still holds, which concludes the proof. □

With these tools at hand, we are now ready to pose appropriate conditions for hand, we are now ready to prove the weak-weak* continuity of $\mathcal{G}$ under the following assumptions:

Assumption 3.51: Conditions for the boundedness and weak-weak*-continuity of $\mathcal{G}$

- The function ρ is at most affine.
- All reaction terms r_a are affine functions.
- The cut-off functions $\phi_c(\cdot) = \phi(e_c^{ret}, \cdot)$ are defined on the whole real line $\mathbb{R}$, and globally Lipschitz continuous.

3.52 Theorem (Continuity and boundedness of $\mathcal{G}$)

Let ASSUMPTION 3.51 hold true. Then, the operator $\mathcal{G} : \mathcal{U} \times \mathcal{Y} \to \mathcal{Z}^\star$ is bounded and weak-weak*-continuous.

Proof. In view of our comment (3.240) at the end of SECTION 3.3.1, it is sufficient to treat each component of $\mathcal{G}$ separately.
We start with the advection operators $\mathcal{G}_a^{adv}$ defined in (3.216). The linear operators $\frac{d}{dt}$ and ∂_x both define bounded, linear mappings with values in $L^2(I_t, H^1(\Omega)^\star)$. We apply LEMMA 3.50, where we choose ϕ to be the identity operator, $y \equiv 1$ in the first case, and $y = v$ in the second one. Since the reaction term r_a is assumed to be affine, the resulting Nemitskii operator is affine as well, and we can again apply LEMMA 3.50 with ϕ being the identity, and $y \equiv 1$.
Next, we examine the hydraulic operators $\mathcal{G}_a^{hyd}$ defined in (3.223). It is sufficient to consider the non-linear part, which we rewrite as

$$\int_{I_t} \left(g\frac{\Delta h_a}{L_a} + \frac{\lambda_a}{2d_a} v_a |v_a|(t) \right) \langle \rho(e_a)(t), z_a^{adv}(t)\rangle_{H^1(\Omega)^\star, H^1(\Omega)} \, dt, \tag{3.273}$$

to better fit our notation. Sicne ρ is assumed to be (at most) affine, we can immediately apply LEMMA 3.50 with $\phi = \left(g\frac{\Delta h_a}{L_a} + \frac{\lambda_a}{2d_a} v_a |v_a|(t) \right)$.
For the initial and boundary conditions, fluxes, and coupling conditions defined in (3.225)-(3.233), the statement follows immediately from LEMMA 3.46 - LEMMA 3.49, and LEMMA 3.38.
□

3.3.3 Fréchet differentiability of $\mathcal{G}$

We complete the analysis of $\mathcal{G}$ by proving its differentiability. Therefore, we briefly recall two common notions of differentiability for operators between Banach spaces. We refer to [Hinze et al., 2009], and [Troeltzsch, 2009], for further reading on this topic in the context of optimization, and [Amann and Escher, 2006] for further reading on the differentiability of operators between the spaces of Banach-valued functions of the class $C^k(I_t, X)$.

3.53 Definition (Fréchet and Gâteaux derivatives)

Let X, Y be two Banach spaces, and $G : U \subset X \to Y$ be an operator defined on an non-empty subset of X.
*Then G is called **Gâteaux differentiable** at x, if the limits*

$$dG(x,h) = \lim_{t \searrow 0} \frac{G(x+th) - G(x)}{t} \in Y \tag{3.274}$$

*exist for all directions $h \in X$, and call $G' : h \mapsto dG(x,h)$ the **Gâteaux derivative** of G in the point x.*
G is called Fréchet differentiable a x, if there exists a continuous, linear operator

$$\mathfrak{D}_x G(x) : X \to Y \tag{3.275}$$

such that

$$\frac{\|G(x+h) - G(x) - \mathfrak{D}_x G(x)h\|_Y}{\|h\|_X} \to 0 \text{ as } \|h\|_X \to 0. \tag{3.276}$$

for all $h \in X$.
If G is Gâteaux/Fréchet differentiable at every point $x \in U$, then we simply call G Gâteaux/Fréchet differentiable. We call G continuously Fréchet differentiable, if the mapping $x \mapsto \mathfrak{D}_x G(x)$ is continuous at every point x.

Both, the structure of the state space $\mathcal{Y}$, and the construction of $\mathcal{G}$, are based on finite Cartesian products. This structure makes it easier to analyse the existence and structure of $\mathfrak{D}\mathcal{G}$. Let

$$F_0 : \mathcal{Y} \to \mathcal{Z}_0 \tag{3.277}$$

be a bounded, continuous, and (continuously) Fréchet differentiable operator between Hilbert spaces, where $\mathcal{Y} = \prod_{i \in I} \mathcal{Y}_i$ is the Cartesian product of finitely many Hilbert spaces. The Fréchet derivative of F_0 at $\bar{y}$ can be expressed as a sum of linear operators

$$\mathfrak{D}_{\mathbf{y}} F_0(\bar{\mathbf{y}})\delta\mathbf{y} = \sum_i \mathfrak{D}_{\mathbf{y}_i} F_0(\bar{\mathbf{y}})\delta\mathbf{y}_i. \tag{3.278}$$

such that it is sufficient to examine each individual component separately, *if all partial derivatives are continuous*. Similarly, if $\mathcal{Z} = \prod_{j \in J} \mathcal{Z}_j$ is a product of Hilbert spaces, and

$$F : \mathcal{Y} \to \mathcal{Z}, F(\mathbf{y}) = \prod_j F_j(\mathbf{y}) \tag{3.279}$$

is the Cartesian product if operators

$$F_j : \mathcal{Y} \to \mathcal{Z}_j, \tag{3.280}$$

its Fréchet derivative (if it exists) can be broken down into the components

$$\mathfrak{D}_{\mathbf{y}} F(\bar{\mathbf{y}})\delta\mathbf{y} = \prod_j \left(\sum_i \mathfrak{D}_{\mathbf{y}_i} F_j(\bar{\mathbf{y}})\delta\mathbf{y}_i \right). \tag{3.281}$$

Therefore, in order to proof that $\mathcal{G}$ is, in fact, continuously Fréchet differentiable, it is both necessary and sufficient to show, that each partial derivative of each component operator exists and is continuous.

Remark 3.54: Generalized gradient

If the spaces $\mathcal{Y}_i$ and $\mathcal{Z}_0$ are separable Hilbert spaces, we observe that for every linear functional $z_0^\star \in \mathcal{Z}_0^\star$ of the Fréchet derivative of F_0, we can rewrite the action of $z_0^\star$ by

$$\begin{aligned} \langle z_0^\star, \mathfrak{D}_{\mathbf{y}} F_0(\bar{\mathbf{y}})\delta\mathbf{y}\rangle_{\mathcal{Z}_0^\star,\mathcal{Z}_0} &= \left\langle z_0^\star, \sum_i \mathfrak{D}_{\mathbf{y}_i} F_0(\bar{\mathbf{y}})\delta\mathbf{y}_i \right\rangle_{\mathcal{Z}_0^\star,\mathcal{Z}_0} \\ &= \sum_i \langle z_0^\star, \mathfrak{D}_{\mathbf{y}_i} F_0(\bar{\mathbf{y}})\delta\mathbf{y}_i\rangle_{\mathcal{Z}_0^\star,\mathcal{Z}_0} \\ &= \sum_i \left\langle \left(\mathfrak{D}_{\mathbf{y}_i} F_0(\bar{\mathbf{y}})\right)^\star z_0^\star, \delta\mathbf{y}_i \right\rangle_{\mathcal{Y}_i^\star,\mathcal{Y}_i} \\ &= \left\langle \prod_i \left(\mathfrak{D}_{\mathbf{y}_i} F_0(\bar{\mathbf{y}})\right)^\star z_0^\star, \delta\mathbf{y} \right\rangle_{\mathcal{Y}^\star,\mathcal{Y}}, \end{aligned} \tag{3.282}$$

and obtain a linear functional in $\mathcal{Y}^\star$. By the Riesz-Fréchet theorem, this functional can be identified with a unique vector $\nabla_{\mathbf{y}}^{z_0} F(\bar{\mathbf{y}}) \in \mathcal{Y}$, such that

$$\begin{aligned} \langle z_0^\star, \mathfrak{D}_{\mathbf{y}} F_0(\bar{\mathbf{y}})\delta\mathbf{y}\rangle_{\mathcal{Z}_0^\star,\mathcal{Z}_0} &= \left(\nabla_{\mathbf{y}}^{z_0} F(\bar{\mathbf{y}}), \delta\mathbf{y}\right)_{\mathcal{Y}} \\ &= \sum_i \left(\nabla_{\mathbf{y}_i}^{z_0} F(\bar{\mathbf{y}}), \delta\mathbf{y}_i\right)_{\mathcal{Y}_i}, \end{aligned} \tag{3.283}$$

and the norm

$$\sup_{\delta\mathbf{y}\in\mathcal{Y}} \left| \langle z_0^\star, \mathfrak{D}_{\mathbf{y}} F_0(\bar{\mathbf{y}})\delta\mathbf{y}\rangle_{\mathcal{Z}_0^\star,\mathcal{Z}_0} \right| = \left\| \nabla_{\mathbf{y}} F(\bar{\mathbf{y}}) \right\|_{\mathcal{Y}} \tag{3.284}$$

is preserved. We can formally identify this process with the operator

$$\left(\tilde{\nabla}_{\mathbf{y}} F(\bar{\mathbf{y}})\right)^\star = \begin{bmatrix} \left(\mathfrak{D}_{\mathbf{y}_0} F_0(\bar{\mathbf{y}})\right)^\star \\ \vdots \\ \left(\mathfrak{D}_{\mathbf{y}_{n_i}} F_0(\bar{\mathbf{y}})\right)^\star \end{bmatrix} \in \prod_i \mathfrak{L}\left(\mathcal{Z}_0^\star, \mathcal{Y}_i^\star\right) \tag{3.285}$$

such that

$$\langle z^\star, \mathfrak{D}_{\mathbf{y}} F_0(\bar{\mathbf{y}})\delta\mathbf{y}\rangle_{\mathcal{Z}_0^\star,\mathcal{Z}_0} = \left(\nabla_{\mathbf{y}}^{z} F(\bar{\mathbf{y}}), \delta\mathbf{y}\right)_{\mathcal{Y}} = \left\langle \left(\tilde{\nabla}_{\mathbf{y}} F(\bar{\mathbf{y}})\right)^\star z^\star, \delta\mathbf{y} \right\rangle_{a^\star,a} \tag{3.286}$$

for *every* linear functional $z^\star \in \mathcal{Z}_0^\star$.

Before we rigorously prove the differentiability of $\mathcal{G}$, we are going to formally derive expressions for each partial derivative, and prove their correctness afterwards. We assume, that $(\bar{\mathbf{u}}, \bar{\mathbf{y}})$ is a solution of $\mathcal{G}(\bar{\mathbf{u}}, \bar{\mathbf{y}}) = 0$, and denote the variation of each state variable $\bar{y}_i$ by y_i (i.e. without a $\bar{\cdot}$ annotation).

For the advection operators we obtain

$$\begin{aligned}\left\langle \mathfrak{D}_{\mathbf{y}}\mathcal{G}_a^{adv}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{y},\mathbf{z}\right\rangle_{\mathcal{Z}^\star,\mathcal{Z}} &= \int_{I_t}\left\langle \frac{d}{dt}e_a(t), z_a^{adv}(t)\right\rangle_{H^1(\Omega_a)^\star,H^1(\Omega_a)} dt \\ &+ \int_{I_t}\left(v_a(t)\partial_x\bar{e}_a(t), z_a^{adv}(t)\right)_{L^2(\Omega_a)} dt \\ &+ \int_{I_t}\left(\bar{v}_a(t)\partial_x e_a(t), z_a^{adv}(t)\right)_{L^2(\Omega_a)} dt \\ &+ \int_{I_t}\left(r_a'\left(\bar{e}_a\right)(t)e_a(t), z_a^{adv}(t)\right)_{L^2(\Omega_a)} dt,\end{aligned} \tag{3.287}$$

as it only depends on the state variables e_a and v_a. Here we observe, that the variation e_a obeys an advection equation with known velocity $\bar{v}_a$, and a linear source term, whereas the variation v_a only appears as a (linear) right hand side of the system.
Similarly, the derivatives of the hydraulic operators $\mathcal{G}_a^{hyd}$ are given by

$$\begin{aligned}\left\langle \mathfrak{D}_{\mathbf{y}}\mathcal{G}_a^{hyd}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{y},\mathbf{z}\right\rangle_{\mathcal{Z}^\star,\mathcal{Z}} &= \int_{I_t}\left(p_{o(a)}(t)-p_{i(a)}(t)\right)z_a^{hyd}(t)\,dt \\ &+ \int_{I_t}\left(g\frac{\Delta h_a}{L_a}+\frac{\lambda_a}{2d_a}\bar{v}_a(t)\left|\bar{v}_a(t)\right|\right)\left(\rho'\left(\bar{e}_a\right)(t)e_a(t), z_a^{hyd}(t)\right)_{L^2(\Omega_a)} dt \\ &+ \int_{I_t}\left(\frac{\lambda_a}{d_a}\left|\bar{v}_a(t)\right|v_a(t)\right)\left(\rho\left(\bar{e}_a\right)(t), z_a^{hyd}(t)\right)_{L^2(\Omega_a)} dt.\end{aligned} \tag{3.288}$$

For the derivatives of fluxes, coupling, initial, and boundary conditions we are going to but have to keep in mind, that the object of concern is actually an element of $\mathrm{Lin}(\mathcal{Y},\mathcal{Z}^\star)$. To give an example, the notation

$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_a^{q:in}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{y} = \left(q_{a:in}+v_aA_a\right)z_a^{q:in} \tag{3.289}$$

should be interpreted in terms of the dual pairing

$$\left\langle \mathfrak{D}_{\mathbf{y}}\mathcal{G}_a^{q:in}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{y},\mathbf{z}\right\rangle_{\mathcal{Z}^\star,\mathcal{Z}} = \int_{I_t}\left(q_{a:in}(t)+v_a(t)d_a\right)z_a^{q:in}(t)\,dt. \tag{3.290}$$

With this notation in mind, we can (formally) formulate operator expressions for the Fréchet derivatives of initial and boundary conditions

$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_a^{e:init}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{y} = e_a(t_0), \tag{3.291}$$

$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_a^{e:in}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{y} = e_{a:in}-e_{i(a)}, \tag{3.292}$$

and the mass and energy fluxes

$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_a^{q:in}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{y} = \left(q_{a:in}+v_aA_a\right), \tag{3.293a}$$

$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_a^{q:out}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{y} = \left(q_{a:in}-v_aA_a\right), \tag{3.293b}$$

$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_a^{Q:in}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{y} = Q_{a:in}-q_{a:in}\bar{e}_{a:in}-\bar{q}_{a:in}e_{a:in}, \tag{3.293c}$$

$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_a^{Q:out}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{y} = Q_{a:out}-q_{a:out}\bar{e}_{a:out}-\bar{q}_{a:out}e_{a:out}, \tag{3.293d}$$

for each pipeline $a\in\mathcal{A}_P$.
Here we want to remind the reader, that $e_{a:in}, e_{a:out}, \bar{e}_{a:in}$, and $\bar{e}_{a:out}$ are compaction notations for the application of the trace operator on e_a and $\bar{e}_a$.

In the same way, we can formulate the derivatives of fluxes and coupling conditions

$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_c^{Q:in}(\bar{\mathbf{u}},\bar{\mathbf{y}}) = Q_{c:in} - q_{c:in}\phi_c\big(\bar{e}_{i(c)}\big) - \bar{q}_{c:in}\phi_c'\big(e_{i(c)}\big), \tag{3.294a}$$
$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_c^{Q:out}(\bar{\mathbf{u}},\bar{\mathbf{y}}) = Q_{c:out} - q_{c:out}e_c^{ret}, \tag{3.294b}$$
$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_c^{\Delta\hat{q}}(\bar{\mathbf{u}},\bar{\mathbf{y}}) = \rho\left(\phi_c(\bar{e}_{i(c)})\right)q_{c:in} + \phi_c'\big(e_{i(c)}\big)\rho'\big(\phi_c\big(e_{i(c)}\big)\big)\bar{q}_{c:in} + \rho\left(e_c^{ret}\right)q_{c:out}, \tag{3.294c}$$
$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_c^{\Delta Q}(\bar{\mathbf{u}},\bar{\mathbf{y}}) = Q_{c:in} + Q_{c:out}, \tag{3.294d}$$

for each consumer $c \in \mathcal{A}_C$, and the producer

$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_s^{Q:in}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{y} = Q_{s:in} - \bar{q}_{s:in}e_{i(s)} - q_{s:in}\bar{e}_{i(s)}, \tag{3.295a}$$
$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_s^{Q:out}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{y} = Q_{s:in} - q_{s:out}\bar{u}_s^e, , \tag{3.295b}$$
$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_s^{p_0}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{y} = p_{i(s)}, \tag{3.296a}$$
$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_s^{\Delta p}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{y} = p_{o(s)} - p_{i(s)}. \tag{3.296b}$$

Finally, the Fréchet derivatives of the flux balance laws w.r.t. $\mathbf{y}$ are given by

$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_N^{\Delta\hat{q}}(\bar{\mathbf{u}},\bar{\mathbf{y}}))\mathbf{y} = \sum_{a\in\mathcal{I}(n)} \rho(\bar{e}_{a:n})q_{a:n} + \bar{q}_{a:n}\rho'(\bar{e}_{a:n})e_{a:n} \tag{3.297a}$$
$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}_n^{\Delta Q}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{y} = \sum_{a\in\mathcal{I}(n)} \bar{e}_{a:n}q_{a:n} + \bar{q}_{a:n}e_{a:n} \tag{3.297b}$$

for each node $n \in \mathcal{N}$. Computing the derivative of $\mathcal{G}$ with respect to the control input $\mathbf{u}$ is way simpler, since only the producer's equations explicitly depend on $\mathbf{u}$. Therefore, we have

$$\mathfrak{D}_{\mathbf{u}}\mathcal{G}_s^{q:in}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{u} = 0, \tag{3.298a}$$
$$\mathfrak{D}_{\mathbf{u}}\mathcal{G}_s^{q:out}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{u} = -u_s^e, \tag{3.298b}$$
$$\mathfrak{D}_{\mathbf{u}}\mathcal{G}_s^{p_0}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{u} = -u_s^{p_0}, \tag{3.299a}$$
$$\mathfrak{D}_{\mathbf{u}}\mathcal{G}_s^{\Delta p}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{u} = -u_s^{\Delta p}, \tag{3.299b}$$

and $\mathfrak{D}_{\mathbf{u}}\mathcal{G}_{a,c}^{\cdots}(\bar{\mathbf{u}},\bar{\mathbf{y}})\mathbf{u} = 0$ for every other equation and component.
Now that we know the rough structure of the linearized operators $\mathfrak{D}_{\mathbf{y}}\mathcal{G}$ and $\mathfrak{D}_{\mathbf{u}}\mathcal{G}$, we are going to show the formal steps leading to (3.287)-(3.299) are, in fact, valid, and the formal system above defines set of bounded, linear operators. We proceed structurally in the same way as we did in SECTION 3.3.2.
As we have already noticed during the analysis of continuity properties, most components of $\mathcal{G}$ are made up of bilinear terms, and compositions with affine or Lipschitz functions. That's why we start with the following observation:

3.55 Lemma (Differentiability of bilinear operators)

Let $(X_1, \|\cdot\|_{X_1})$, $(X_2, \|\cdot\|_{X_2})$, and $(Y, \|\cdot\|_Y)$ be Banach spaces and $B : X_1 \times X_2 \to Y$ a bounded, bilinear operator. Then B is continuously Fréchet differentiable with derivative

$$B'(\bar{x}_1,\bar{x}_2)h = B(\bar{x}_1,h_2) + B(h_1,\bar{x}_2). \tag{3.300}$$

Proof. We proceed similarly as is in the proof given in [Hinze et al., 2009], but fill in a few details. Let $t > 0$ and $h \in X_1 \times X_2 := X$. Since B is bilinear, we have

$$B(\bar{x}_1 + th_1, \bar{x}_2 + th_2) - B(\bar{x}_1,\bar{x}_2) = t^2B(h_1,h_2) + tB(\bar{x}_1,h_2) + tB(h_1,\bar{x}_2), \tag{3.301}$$

such that we can easily compute the Gâteaux derivative

$$\lim_{t\to 0}\frac{B(\bar{x}_1 + th_1, \bar{x}_2 + th_2) - B(\bar{x}_1,\bar{x}_2)}{t} = B(\bar{x}_1,h_2) + B(h_1,\bar{x}_2). \tag{3.302}$$

The partial evaluations $B(\bar{x}_1, \cdot)$ and $B(\cdot, \bar{x}_2)$ are linear operators, because B is bilinear and bounded by assumption, For the remainder term

$$B(\bar{x}_1 + h_1, \bar{x}_2 + h_2) - B(\bar{x}_1, \bar{x}_2) - B'(\bar{x}_1, \bar{x}_2)h = B(h_1, h_2) \tag{3.303}$$

we use the estimate

$$\|B(h_1, h_2)\|_Y \leq \|B\| \, \|h_1\|_{X_1} \, \|h_2\|_{X_2} \leq \|B\| \, \|h\|_X^2 \tag{3.304}$$

and conclude that B is in fact Fréchet differentiable, since

$$0 \leq \lim_{\|h\| \to 0} \frac{\|B(h_1, h_2)\|_Y}{\|h\|_X} \leq \lim_{\|h\| \to 0} \frac{\|B\| \, \|h\|_X^2}{\|h\|_X} = 0. \tag{3.305}$$

Finally, we use the explicit formula for $\mathfrak{D}_x B(\bar{x})$, and boundedness of B to derive the estimate

$$\|\mathfrak{D}_x B(\bar{x})h\|_Y \leq \|B\| \left(\|\bar{x}_1\|_{X_1} \, \|h_1\|_{X_1} + \|\bar{x}_2\|_{X_2} \, \|h_2\|_{X_2} \right) \leq \|B\| \, \|\bar{x}\|_X^2 \, \|h\|_X^2 \tag{3.306}$$

such that $\mathfrak{D}_x B(\bar{x})$ is bounded and therefore continuous with respect to $\bar{x} = (\bar{x}_1, \bar{x}_2)$. □

3.56 Lemma (Fréchet differentiability of Nemitskii operators I)

Let $\phi : \mathbb{R} \to \mathbb{R}$ be continuously differentiable, with globally Lipschitz continuous derivative. Then the operator

$$\begin{aligned} N_\phi &: H^1(I_t) \to H^1(I_t)^\star \\ \langle N_\phi(y), z \rangle_{H^1(I_t)^\star, H^1(I_t)} &= \int_{I_t} \phi(y) z(t) \, dt, \end{aligned} \tag{3.307}$$

which has already been introduced in LEMMA 3.46 *, is continuously Fréchet differentiable, where its derivative at $\bar{y} \in H^1(I_t)$ is given by the bounded, linear operator*

$$\begin{aligned} \mathfrak{D}_y N_\phi &: H^1(I) \to H^1(I)^\star \\ \langle \mathfrak{D}_y N_\phi(\bar{y}) y, z \rangle_{H^1(I_t)^\star, H^1(I_t)} &\coloneqq \int_{I_t} \phi'(\bar{y})(t) y(t) z(t) \, dt. \end{aligned} \tag{3.308}$$

Proof. We already know, that N_ϕ is continuous and bounded by LEMMA 3.46 .
First, we consider the restriction

$$\phi^\sharp : C^0(\bar{I}_t) \to C^0(\bar{I}_t), y \mapsto \phi \circ y \tag{3.309}$$

of ϕ, which is continuously differentiable (see e.g. [Amann and Escher, 2006], chapter 7). Its derivative $\mathfrak{D}_y N_\phi^\sharp \in \mathrm{Lin}\big(C^0(\bar{I}_t), C^0(\bar{I}_t)\big)$ is given by

$$\mathfrak{D}_y \phi^\sharp(\bar{y})(t) \cdot \delta y(t) = \phi'(\bar{y}) \delta y. \tag{3.310}$$

If we utilize the (continuous) embeddings of $H^1(I_t)$, into $C^0(\bar{I}_t)$ and $C^0(\bar{I}_t)$ into $H^1(I_t)^\star$, we find that the corresponding weak formulation

$$\begin{aligned} N_\phi^\sharp &: C^0(\bar{I}_t) \to H^1(I_t)^\star \\ \left\langle N_\phi^\sharp(y), z \right\rangle_{H^1(I_t)^\star, H^1(I_t)} &\coloneqq \int_{I_t} \phi(y)(t) z(t) \, dt \end{aligned} \tag{3.311}$$

is also well defined and continuously Fréchet differentiable, with

$$\left\langle \mathfrak{D}_y N_\phi^\sharp(\bar{y})y, z \right\rangle_{H^1(I_t)^\star, H^1(I_t)} := \int_{I_t} \phi'(\bar{y})(t)y(t)z(t)\,dt. \tag{3.312}$$

Furthermore, this operator is well defined for $\bar{y} \in H^1(I)$, bounded and weak-weak*-continuous (hence continuous) in both arguments by LEMMA 3.46 and LEMMA 3.47. To be more precise, we have that

$$\left|\left\langle \mathcal{D}_y N_\phi^\sharp(\bar{y})y, z \right\rangle\right| \leq C \cdot \|z\|_{H^1(I_t)} \cdot \|y\|_{H^1(I)} \cdot \left|\int_{I_t} \phi'(\bar{y})(t)\,dt\right| < \infty \tag{3.313}$$

such that its operator norm

$$\left\|\mathcal{D}_y N_\phi^\sharp\right\|_{H^1(I_t)^\star} = \sup_{\|z\|\leq 1} \sup_{\|\delta x\|\leq 1} |\langle \mathcal{D}_y N_\phi(\bar{x}, \bar{y})\delta x, z\rangle| < \infty \tag{3.314}$$

is finite. It remains to show, that our candidate $\mathcal{D}_y N_\phi^\sharp$ is, in fact, the Fréchet derivative of N_ϕ. This, follows immediately from the continuity properties of N_ϕ, $N_\phi^\sharp$, and $\mathcal{D}_y N_\phi^\sharp$, together with the standard density argument for H^1 functions. □

The remaining statements, which represent the differentiability statements analogous to LEMMA 3.49 - LEMMA 3.50, are direct consequences of LEMMA 3.56, LEMMA 3.55, and the *chain rule for Fréchet differentiable mappings*.

3.57 Lemma (Fréchet differentiability of Nemitskii operators II)

Let $(X, \|\cdot\|_X)$ be a Banach space, and $A : X \to L^2(I_t)$ a continuous, affine operator. Then the operator $B : X \times H^1(I_t) \to H^1(I_t)^\star$

$$\langle B(x, y), z\rangle_{H^1(I_t)^\star, H^1(I_t)} = \int_{I_t} (Ax)(t)y(t)z(t)\,dt, \tag{3.315}$$

defined in LEMMA 3.49 is continuously Fréchet differentiable with partial derivatives

$$\langle \mathfrak{D}_x B(\bar{x}, \bar{y})x, z\rangle_{H^1(I_t)^\star, H^1(I_t)} = \int_{I_t} (Lx)(t)x(t)\bar{y}(t)z(t)\,dt, \tag{3.316a}$$

$$\langle \mathfrak{D}_y B(\bar{x}, \bar{y})y, z\rangle_{H^1(I_t)^\star, H^1(I_t)} = \int_{I_t} (A\bar{x})(t)y(t)z(t)\,dt, \tag{3.316b}$$

where L is the (bounded) linear part of A.

Proof. The affine operator A is (infinitely often) continuously Fréchet differentiable with derivative $\mathfrak{D}_x A = L$.
The operator $(x, y) \mapsto (Ax) \cdot y$ is bilinear, such that the statement about the partial derivatives follows from LEMMA 3.55 and the chain rule for Fréchet derivatives.
Both partial derivatives are bounded linear operators, and weak-weak*-continuous w.r.t. $\bar{x}$ and $\bar{y}$. Therefore, B is continuously Fréchet differentiable. □

3.58 Lemma (Fréchet differentiability of Nemitskii operators III)

Let $(X, \|\cdot\|_X)$ be a real Banach space, $Y = H^1(I_t)$, and $A : X \to L^2\big(I_t, H^1(\Omega)^\star\big) =: Z^\star$ a continuous, affine operator, and $\phi : \mathbb{R} \to$ is continuously differentiable with Lipschitz continuous derivative. Then the operator

$$\langle B(x,y), z\rangle_{Z^\star,Z} := \int_{I_t} \phi(y)(t) \cdot \langle A\,(x)\,(t), z(t)\rangle_{H^1(\Omega)^\star,H^1(\Omega)}\, dt, \tag{3.317}$$

defined in LEMMA 3.50 *is continuously Fréchet differentiable. Its partial derivatives are given by the linear operators*

$$\langle \mathfrak{D}_x B(\bar{x},\bar{y})x, z\rangle_{H^1(I_t)^\star,H^1(I_t)} = \int_{I_t} \phi(\bar{y})(t)\, \langle Lx(t), z(t)\rangle_{H^1(\Omega)^\star,H^1(\Omega)}\, dt, \tag{3.318a}$$

$$\langle \mathfrak{D}_y B(\bar{x},\bar{y})y, z\rangle_{H^1(I_t)^\star,H^1(I_t)} = \int_{I_t} \phi'(\bar{y})(t)\, \langle A\,(\bar{x})\,(t), z(t)\rangle_{H^1(\Omega)^\star,H^1(\Omega)}\, y(t)\, dt. \tag{3.318b}$$

Proof. Like in the proof of LEMMA 3.57, the statement follows from a combination of LEMMA 3.55, the chain rule, and the continuity properties derived from LEMMA 3.47 and LEMMA 3.50. □

By combining the results above, we can extend ASSUMPTION 3.51, such that we can prove the differentiability of $\mathcal{G}$.

Assumption 3.59: Conditions for the Fréchet differentiability of $\mathcal{G}$

In addition to ASSUMPTION 3.51, we assume that for every consumer $c \in \mathcal{A}_C$, the cut-off function $\phi_c : \mathbb{R} \to \mathbb{R}$ is continuously differentiable, with globally Lipschitz continuous derivative.

3.60 Theorem (Differentiability of $\mathcal{G}$)

Let ASSUMPTION 3.59 *hold true. Then, $\mathcal{G}$ is continuously Fréchet differentiable, where the derivatives*

$$\mathcal{D}_{\mathbf{u}}\mathcal{G} \in C^0(\mathcal{U} \times \mathcal{Y}, \mathrm{Lin}(\mathcal{U}, \mathcal{Z}^\star)), \tag{3.319}$$

and

$$\mathcal{D}_{\mathbf{y}}\mathcal{G} \in C^0(\mathcal{U} \times \mathcal{Y}, \mathrm{Lin}(\mathcal{Y}, \mathcal{Z}^\star)), \tag{3.320}$$

are given by the expressions (3.287)-(3.299).

Proof. We proceed analogously to the proof of THEOREM 3.52, and begin with the advection-reaction operators $\mathcal{G}_a^{adv}$. The operator $\frac{d}{dt}$ is linear and bounded, such that it is automatically continuously differentiable. The convection term is handled by LEMMA 3.58, and the reaction term is affine, and therefore differentiable, where the derivative is the Nemitskii operator generated by the function $r_a'(\cdot)$.

For the hydraulic operators $\mathcal{G}_a^{hyd}$

$$\int_{I_t} \left(g \frac{\Delta h_a}{L_a} + \frac{\lambda_a}{2d_a} v_a \left| v_a \right| (t) \right) \left\langle \rho \left(e_a \right) (t), z_a^{adv}(t) \right\rangle_{H^1(\Omega)^\star, H^1(\Omega)} \, dt, \tag{3.321}$$

we recognize that the first term is differentiable with Lipschitz derivative, and the second one is affine w.r.t. e_a, such that this operator fits the prerequisites of LEMMA 3.58 .
For the fluxes and coupling conditions of nodes, consumers and the producer, the differentiability statement follows immediately from LEMMA 3.56 , LEMMA 3.55 , and the chain rule.
The differentiability of the fluxes, initial and boundary conditions is obtained by a combination LEMMA 3.57 , LEMMA 3.55 , and the chain rule.

□

3.3.4 The linearized residual operator

We summarize the previous result on one page. We assume that $\bar{\mathbf{y}}, \bar{\mathbf{u}}$ is a solution of $\mathcal{G}(\bar{\mathbf{y}}, \bar{\mathbf{u}}) = 0$, and all variables, which are not marked with a $\bar{\cdot}$ are their variations in their corresponding Hilbert space. Let $\mathcal{F} \in \mathcal{Z}^\star$. Then $\mathfrak{D}_{\mathbf{y}}\mathcal{G}(\bar{\mathbf{y}}, \bar{\mathbf{u}})\mathbf{y} = \mathcal{F}$ is equivalent to the weak formulation of the following system of linear equations:
For each pipe $a \in \mathcal{A}_P$, we solve the linearized advection-reaction and pressure difference equations

$$\partial_t e_a + \bar{v}_a \partial_x e_a + r_a'\left(\bar{e}_a\right) e_a, = -v_a \partial_x \bar{e}_a + \mathcal{F}_a^{adv} \tag{3.322a}$$

$$p_{o(a)} - p_{i(a)} = -\left(g\frac{\Delta h_a}{L_a} + \frac{\lambda_a}{2d_a}\bar{v}_a\left|\bar{v}_a\right|\right)\int_{\Omega_a}\rho'\left(\bar{e}_a\right)e_a\,dx - \frac{\lambda_a}{2d_a}\left|\bar{v}_a\right|v_a\int_{I_t}\rho\left(\bar{e}_a\right)(t)\,dx + \mathcal{F}_a^{hyd}, \tag{3.322b}$$

$$e_{a:in} = e_{i(a)} + \mathcal{F}_a^{e:in}, \tag{3.322c}$$

$$e_a(t_0) = \mathcal{F}_a^{init}, \tag{3.322d}$$

which are supplemented by the appropriate linearized initial and boundary conditions. The corresponding linearized fluxes are given as the solutions of

$$q_{a:in} = -A_a v_a + \mathcal{F}_a^{q:in}, \tag{3.323a}$$

$$q_{a:out} = A_a v_a + \mathcal{F}_a^{q:out}, \tag{3.323b}$$

$$Q_{a:in} = q_{a:in}\bar{e}_{a:in} + \bar{q}_{a:in}e_{a:in} + \mathcal{F}_a^{Q:in}, \tag{3.324a}$$

$$Q_{a:out} = q_{a:out}\bar{e}_{a:out} + \bar{q}_{a:out}e_{a:out} + \mathcal{F}_a^{Q:out}. \tag{3.324b}$$

For each consumer $c \in \mathcal{A}_C$, the linearized fluxes and balance conditions are given by

$$\rho\left(\bar{e}_{i(c)}\right)q_{c:in} + \rho'\left(\bar{e}_{i(c)}\right)e_{i(c)}\bar{q}_{c:in} = -\rho\left(\bar{e}_{o(c)}\right)q_{c:out} + \rho'\left(\bar{e}_{o(c)}\right)e_{o(c)}\bar{q}_{c:out} + \mathcal{F}_c^{\Delta\hat{q}}, \tag{3.325a}$$

$$Q_{c:in} = q_{c:in}\phi\left(e_c^{min}, \bar{e}_{i(c)}\right) + \bar{q}_{c:in}\phi'\left(e_c^{min}, \bar{e}_{i(c)}\right)e_{i(c)} + \mathcal{F}_c^{\Delta Q}, \tag{3.325b}$$

$$Q_{c:out} = q_{c:out}e_c^{ret} + \mathcal{F}_c^{q:out}, \tag{3.325c}$$

$$Q_{c:in} + Q_{c:out} = \mathcal{F}_c^{q:out}. \tag{3.325d}$$

For the producer s, the linearized energy fluxes and hydraulic coupling conditions are

$$Q_{s:in} = \bar{q}_{s:in}e_{i(s)} + q_{s:in}\bar{e}_{i(s)} + \mathcal{F}_a^{q:in}, \tag{3.326a}$$

$$Q_{s:out} = \bar{q}_{s:out}u^e + q_{s:out}\bar{u^e} + \mathcal{F}_s^{q:out}, \tag{3.326b}$$

$$p_{i(s)} = \mathcal{F}_s^{p_0}, \tag{3.326c}$$

$$p_{o(s)} - p_{i(s)} = \mathcal{F}_s^{\Delta p}. \tag{3.326d}$$

For each node $n \in \mathcal{N}$, we obtain the following set of linearized flux balance laws

$$\sum_{a\in I_n}\rho'\left(\bar{e}_{a:n}\right)e_{a:n}\bar{q}_{a:n} + \rho\left(\bar{e}_{a:n}\right)q_{a:n} = \mathcal{F}_n^{\Delta\hat{q}}, \tag{3.327}$$

$$\sum_{a\in I_n}Q_{a:n} = \mathcal{F}_n^{\Delta Q}. \tag{3.328}$$

The linearized system has roughly the same structure as the original on given in SECTION 2.6, with the exception that all interactions between thermodynamic and hydraulic variables are either linear or bilinear. In particular, the contributions of variations of velocity v_a to (3.322a) only act as a linear right hand side.

3.3.5 Well-posedness of weak solutions in terms of $\mathcal{G}$

In the previous sections, we have established an abstract residual operator of the model equations, which we have proven to be equivalent to solutions in terms of characteristics. This was motivated by the observation, that the classical function spaces used in the explicit construction of solutions complicate the analysis of optimization problems for district heating networks. In this section, we are going to show that this construction is, in fact, well defined.

3.61 Proposition (Residual operator formulation of the unsteady advection problem)

Consider the unsteady advection problem (3.8) for a single pipeline, and let e be a solution in the sense of PROPOSITION *3.3, where the inflow energy e^{in}, initial energy e^{init}, and flow velocity v are assumed to be known in advance, and fulfil the requirements of* PROPOSITION *3.3. We define $\mathcal{G}^{sp} = \mathcal{G}^{adv} \times \mathcal{G}^{e:in} \times \mathcal{G}^{e:init}$. Then e is an element of $\mathcal{E} = H^1\big(I_t, H^1(\Omega), H^1(\Omega)^\star\big)$ and solves $\langle \mathcal{G}^{sp}, z^{sp}\rangle = 0 \, \forall z \in \mathcal{E} \times H^1(I_t) \times H^1(\Omega)$. This solution is unique, such that both formulations can be seen as equivalent. In particular, solutions of the weak formulation inherit higher regularity properties from the characteristics solution.*

Proof. **Step 1**: Existence.
We are going to show, that the solution e given in SECTION *3.2* is an element of $L^2\big(I_t, H^1(\Omega)\big)$.

By COROLLARY *3.25*, we know that $e \in C^0\big(\bar{I}_t, H^1(\Omega)\big)$.
Therefore, the function

$$f(t) = \langle \phi, e(t)\rangle_{H^1(\Omega)^\star, H^1(\Omega)} \tag{3.329}$$

is continuous and Lebesgue measurable for any linear functional $\phi \in H^1(\Omega)^\star$. Since $H^1(\Omega)$ is separable, we know that e is Bochner measurable by THEOREM *3.33*, and we may estimate its norm by

$$\|e\|_{L^2(I_t, H^1(\Omega))} = \sqrt{\int_{I_t} \|e(t)\|^2_{H^1(\Omega)} \, dt} \leq \sqrt{|I_t|}\, \|e\|_{C^0\left(\bar{I}_t, H^1(\Omega)\right)} < \infty \tag{3.330}$$

such that $e \in L^2\big(I_t, H^1(\Omega)\big)$.
We know that e has partial derivative in the sense of Sobolev spaces, such that the mapping

$$\frac{d}{dt} : t \mapsto \partial_t e(t,\cdot) = -v(t)\partial_x e(t,\cdot) - r(e)(t,\cdot) \tag{3.331}$$

is defined almost everywhere in $I_t \times \Omega$, and by the regularity properties an element of $L^2(I_t \times \Omega) \cong L^2\big(I_t, L^2(\Omega)\big)$.
Finally, the continuous embedding

$$L^2\big(I_t, L^2(\Omega)\big) \hookrightarrow L^2\big(I_t, H^1(\Omega)^\star\big) \tag{3.332}$$

which is a consequence of the Aubin-Lions-Lemma THEOREM *3.41*, such that $\frac{d}{dt} e \in L^2\big(I_t, H^1(\Omega)^\star\big)$.

Step 2: Uniqueness.

Let e_1, e_2 be two solutions of the weak advection-reaction problem, and define $e^\Delta = e_2 - e_1$.

By the linearity of $\mathcal{G}^{init}$ and $\mathcal{G}^{e:in}$, we can assume $e^{\Delta}(t_0) = 0$, $tr_0 e^{\Delta} = 0$, and focus on the advection operator.

We are going to show that $e^{\Delta} \equiv 0$ by using an energy argument.

Since e_1, and e_2 are both weak solutions, and r is assumed to be at most affine, we know that the difference e^{Δ} is a weak solution of the transport equation with linear reaction term, and therefore

$$\begin{aligned}\int_{I_t} \left\langle \frac{d}{dt} e^{\Delta}(s), e^{\Delta}(s) \right\rangle_{H^1(\Omega)^\star, H^1(\Omega)} ds + \int_{I_t} v(s) \left(\partial_x e^{\Delta}(s), e^{\Delta}(s)\right)_{L^2(\Omega)} ds \\ + \int_{I_t} \left(r_1 e^{\Delta}(s), e^{\Delta}(s)\right)_{L^2(\Omega)} = 0,\end{aligned} \tag{3.333}$$

where we chose $z^{adv} = e^{\Delta}$ as our test function. For the convection term, we obtain a rough estimate

$$\begin{aligned}\left| \int_\Omega \partial_x e^{\Delta}(s) \cdot e^{\Delta}(s)\, dx \right| &= \frac{1}{2} \left| \int_\Omega \partial_x e^{\Delta}(s)^2\, dx \right| \\ &\leq \frac{1}{2} \left| \left(e^{\Delta}(s)(L)^2 + e^{\Delta}(s)(0)^2\right) \right| \\ &\leq C_1 \left\| e^{\Delta}(s) \right\|^2_{L^2(\Omega)}\end{aligned} \tag{3.334}$$

for some constant $C_1 > 0$, and almost every $s \in I_t$. The reaction term can be estimated

$$\left| \int_\Omega r_1 e^{\Delta}(s) \cdot e^{\Delta}(s)\, dx \right| \leq C_2 \left\| e^{\Delta}(s) \right\|^2_{L^2(\Omega)} \tag{3.335}$$

for another constant $C_2 > 0$, and almost every $s \in I_t$.

Now we combine these estimates and obtain

$$\frac{d}{dt} \left\| e^{\Delta}(t) \right\|^2_{\mathcal{E}} \leq C \left\| e^{\Delta}(t) \right\|^2_{\mathcal{E}} \tag{3.336}$$

such that by the Gronwall Lemma

$$\left\| e^{\Delta}(t) \right\|^2_{\mathcal{E}} \leq \left\| e^{\Delta}(t_0) \right\|^2_{\mathcal{E}} \exp\left(C(t - t_0)\right) = 0. \tag{3.337}$$

Therefore, $e_1 = e_2$ in the norm of $\mathcal{E}$, and the solution given in *step 1* is unique. □

We conclude this chapter by the following theorem, which summarizes most results of our analysis, and completes the connection with the less abstract results in SECTION 3.1 and SECTION 3.2.

3.62 Theorem (Existence and uniqueness of weak solutions for simple networks)

Let $\mathbf{u} \in \mathcal{U}_{ad} \subseteq \mathcal{U}$. Then there exists a unique solution $\mathbf{y} \in \mathcal{Y}$ in the sense that

$$\langle \mathcal{G}(\mathbf{u}, \mathbf{y}), \mathbf{z} \rangle_{\mathcal{Z}^\star, \mathcal{Z}} = 0 \qquad \forall \mathbf{z} \in \mathcal{Z}. \tag{3.338}$$

This implicitly defines the solution operator

$$\mathcal{S} : \mathcal{U}_{ad} \longrightarrow \mathcal{Y}, \mathcal{G}(\mathbf{u}, \mathbf{y}) = 0 \Leftrightarrow \mathbf{y} = \mathcal{S}(\mathbf{u}) \tag{3.339}$$

which is weak-weak*-continuous, bounded, and injective.
If $(\bar{\mathbf{u}}, \bar{\mathbf{y}})$ is a solution of $\mathcal{G}(\bar{\mathbf{u}}, \bar{\mathbf{y}})$, and if we assume, that $\mathfrak{D}_y \mathcal{G}(\bar{\mathbf{u}}, \bar{\mathbf{y}})$ has a bounded inverse, $\mathcal{S}$ is continuously Fréchet differentiable in an open neighbourhood $\tilde{\mathcal{U}}$ of $\bar{u}$, and its derivative is given by

$$\mathcal{S}'(\bar{\mathbf{u}})\mathbf{u} := \mathfrak{D}_{\mathbf{u}} \mathcal{S}(\bar{\mathbf{u}})\mathbf{u} = \left(\mathfrak{D}_{\mathbf{y}} \mathcal{G}(\bar{\mathbf{u}}, \bar{\mathbf{y}})\right)^{-1} \mathfrak{D}_{\mathbf{u}} \mathcal{G}(\bar{\mathbf{u}}, \bar{\mathbf{y}})\mathbf{u} \tag{3.340}$$

for all $\mathbf{u} \in \tilde{\mathcal{U}}$.

Proof. Existence and uniqueness for the advection problem for a single pipeline with known velocity, initial, and boundary conditions has been proven in PROPOSITION *3.61*. Using a graph traversal argument like in the proof of THEOREM *3.23*, we conclude that the solution given by COROLLARY *3.25* is an element of the state space $\mathcal{Y}$ given in DEFINITION *3.39*, and solves the equation $\mathcal{G}(\mathbf{u}, \mathbf{y}) = 0_{\mathcal{Z}^\star}$.
For uniqueness, we consider an arbitrary solution of $\mathcal{G}(\mathbf{u}, \mathbf{y}) = 0$. The additional regularity of the energy densities e_a implied by PROPOSITION *3.61* ensures the existence of a unique, continuous representative. The discussion preceding the weak formulations of all fluxes, initial, boundary, and coupling conditions in SECTION *3.3.1*, in particular the estimate (3.220), shows that the same holds true for all other state variables. Therefore, this solution must be unique by THEOREM *3.23*.
As a result, the solution operator (or state-to-control mapping) $\mathcal{S}$ is well defined, bounded, and injective, where the boundedness follows from THEOREM *3.52*.
In order to prove weak-weak*-continuity, we consider a weakly convergent sequence $\mathbf{u}_n$ in $\mathcal{U}$, such that $\mathbf{y}_n = \mathcal{S}(\mathbf{u}_n)$ defines a bounded sequence in $\mathcal{Y}$.
Since we know, that $\mathcal{U} \times \mathcal{Y}$ is reflexive, we can extract a weakly convergent subsequence $(\mathbf{u}_{n_k}, \mathbf{y}_{n_k})$. It remains to show, that the weak limit satisfies $\mathbf{y} = \mathcal{S}(\mathbf{u})$, i.e. that it is indeed a solution of $\mathcal{G}(\mathbf{u}, \mathbf{y}) = 0_{\mathcal{Z}^\star}$. THEOREM *3.52* states that $\mathcal{G}$ is weak-weak*-continuous, such that

$$\langle \mathcal{G}(\mathbf{u}_{n_k}, \mathbf{y}_{n_k}), \mathbf{z} \rangle_{\mathcal{Z}^\star, \mathcal{Z}} \to \langle \mathcal{G}(\mathbf{u}, \mathbf{y}), \mathbf{z} \rangle_{\mathcal{Z}^\star, \mathcal{Z}} \qquad \forall \mathbf{z} \in \mathcal{Z}, \tag{3.341}$$

which completes this part the proof. If we additionally assume, that $\mathfrak{D}_y \mathcal{G}$ has a bounded inverse at every solution, the identity (3.340) follows by the implicit function theorem for Banach spaces (see [Hinze et al., 2009]). □

Chapter 4

Applications in optimal control

In this chapter of the thesis, we turn towards optimal control problems built upon the model which we have established in CHAPTER 2, and demonstrate their solution by applying the insights from the analysis in CHAPTER 3.
Given the regularity assumptions of the control input implied by DEFINITION 3.42, we consider the following cost functional

$$\begin{aligned}\mathcal{J}^u(\mathbf{u}) = &\frac{\alpha_0^e}{2}\left\|u^e\right\|_{L^2(I_t)}^2 + \frac{\alpha_1^e}{2}\left\|\partial_t u^e\right\|_{L^2(I_t)}^2 \\ &+ \frac{\alpha_0^p}{2}\left\|u^{p_0}\right\|_{L^2(I_t)}^2 + \frac{\alpha_1^p}{2}\left\|\partial_t u^{p_0}\right\|_{L^2(I_t)}^2 \\ &+ \frac{\alpha_0^{\Delta p}}{2}\left\|u^{\Delta p}\right\|_{L^2(I_t)}^2 + \frac{\alpha_1^{\Delta p}}{2}\left\|\partial_t u^{\Delta p}\right\|_{L^2(I_t)}^2,\end{aligned} \tag{4.1}$$

which seeks to minimize an weighted sum of the average value, and average variation of each control variable.
In view of the regularity results of CHAPTER 3, we can formulate the inequality state constraints listed in SECTION 2.6 as mappings

$$\begin{aligned}\mathcal{C}_c^e(\mathbf{y}) :&\mathcal{Y} \to H^1(I_t)^2 \\ &\mathbf{y} \mapsto \begin{pmatrix} e_c^{min} - e_{i(c)} \\ e_{i(c)} - e_c^{max}\end{pmatrix},\end{aligned} \tag{4.2}$$

$$\begin{aligned}\mathcal{C}_c^p(\mathbf{y}) :&\mathcal{Y} \to H^1(I_t)^2 \\ &\mathbf{y} \mapsto \begin{pmatrix} p_c^{min} - p_{i(c)} \\ p_{i(c)} - p_c^{max}\end{pmatrix},\end{aligned} \tag{4.3}$$

for the box constraints of pressure and energy density at the inflow of each consumer station $c \in \mathcal{A}_C$, and

$$\begin{aligned}\mathcal{C}_c^{\Delta p}(\mathbf{y}) :&\mathcal{Y} \to H^1(I_t)^2 \\ &\mathbf{y} \mapsto \begin{pmatrix} p_c^{min} + p_{i(c)} - p_{o(c)} \\ p_{o(c)} - p_{i(c)} - p_c^{max}\end{pmatrix},\end{aligned} \tag{4.4}$$

$$\begin{aligned}\mathcal{C}_s^{\Delta Q}(\mathbf{y}) :&\mathcal{Y} \to H^1(I_t)^2 \\ &\mathbf{y} \mapsto \begin{pmatrix} \Delta Q^{min} - Q_{s:in} - Q_{s:out} \\ Q_{s:in} + Q_{s:out} - \Delta Q^{max}\end{pmatrix},\end{aligned} \tag{4.5}$$

for pressure difference constraint of each consumer c, and the power constraint of the producer s, and combine them into a single mapping

$$\begin{aligned}\mathcal{C}(\mathbf{y}) :&\mathcal{Y} \to H^1(I_t)^{N_C} \\ &\mathbf{y} \mapsto \mathcal{C}_s^{\Delta Q}(\mathbf{y}) \times \prod_{c \in \mathcal{A}_C} \left(\mathcal{C}_c^e(\mathbf{y}) \times \mathcal{C}_c^p(\mathbf{y}) \times \mathcal{C}_c^{\Delta p}(\mathbf{y})\right),\end{aligned} \tag{4.6}$$

by utilizing the same Cartesian product construction, which we already have used in SECTION 3.3. Here, $N_C = 2 + 6 \cdot |\mathcal{A}_C|$ is the total number of state constraints of the system.

We make use of the following concept, in order to formalize our inequality constraints on abstract spaces:

4.1 Definition (Convex cone)

A subset $\mathcal{K} \subset X$ of a Banach space $(X, \|\cdot\|_X)$ is called ***convex cone****, if*

$$\forall a > 0 : x \in \mathcal{K} \Rightarrow a \cdot x \in \mathcal{K}. \tag{4.7}$$

It is common to adopt the notation

$$x \geq_{\mathcal{K}} 0 \Leftrightarrow x \in \mathcal{K}, \qquad x \leq_{\mathcal{K}} 0 \Leftrightarrow -x \in \mathcal{K}. \tag{4.8}$$

Accordingly, we define the convex cone

$$\mathcal{K}_C = \prod_{i=1}^{6\cdot|\mathcal{A}_C|\cdot} \left\{ z \in H^1(I_t) \,\middle|\, z(t) \geq 0 \forall t \in I_t \right\} \tag{4.9}$$

which is a closed subset of $H^1(I_t)^{6\cdot|\mathcal{A}_C|}$ due to the embedding of $H^1(I_t)$ into $C^0(\bar{I}_t)$.
We refer to [Troeltzsch, 2009], and [Hinze et al., 2009] for a broader overview on the topic of abstract optimization problems in Banach spaces. Combining the pieces above leads to the following optimization problem:

$$P_0 : \quad \begin{cases} \min\limits_{\mathbf{u},\mathbf{y} \in \mathcal{U} \times \mathcal{Y}} \mathcal{J}^u(\mathbf{u}, \mathbf{y}) \\ \text{subject to} \\ \qquad \mathcal{G}(\mathbf{u}, \mathbf{y}) = 0_{\mathcal{Z}^\star}, \\ \qquad \mathcal{C}(\mathbf{y}) \leq_{\mathcal{K}_\mathcal{C}} 0, \\ \qquad u^e \in \mathcal{U}^{ad}. \end{cases} \tag{4.10}$$

where $\mathcal{G}$ is the residual operator defined in SECTION 3.3, $\mathcal{C}$ and $\mathcal{K}_\mathcal{C}$ are defined as above, and $\mathcal{U}^{ad}$ models the box constraints for control variables, as suggested in DEFINITION 3.42.
In the case of our district heating model, we neither guarantee the feasibility of all state constraints, nor provide an initial solution, such that the feasible ones are satisfied. By numbering the constraints in ascending order, we define the index set $\mathcal{I}_\mathcal{C} \subset \{1, \ldots, N_C\}$ of constraints, which we want to regularize. For each $i \in \mathcal{I}_\mathcal{C}$, we select the respective constraint mapping

$$\mathcal{C}_i(\mathbf{y}) = \begin{pmatrix} y_i^{min} - y_i \\ y_i - y_i^{max} \end{pmatrix} \tag{4.11}$$

and replace it by a *Moreau-Yosida* type penalty term

$$\mathcal{J}^{\delta_i}(\mathbf{y}) = \frac{\delta_i}{2} \int_{I_t} \left(\left(y_i^{min} - y_i(t) \right)^+ \right)^2 + \left(\left(y_i(t) - y_i^{max} \right)^+ \right)^2 dt \tag{4.12}$$

where y_i refers to the (linear combinations) of state variables, whom the i^{th} constraint explicit depends on, and $\delta_i \geq 0$ is a possibly large, real parameter.
Given such an index set $\mathcal{I}_\mathcal{C}$, and a parameter vector $\delta \in \mathbb{R}^{|\mathcal{I}_\mathcal{C}|}$, we define the *regularization cost functional*

$$\mathcal{J}^{\mathcal{I}_\mathcal{C}, \delta}(\mathbf{y})) = \sum_{i \in \mathcal{I}_\mathcal{C}} \mathcal{J}^{\delta_i}(\mathbf{y}), \tag{4.13}$$

the *reduced constraint mapping*

$$\mathcal{C}^{\mathcal{I}_c}(\mathbf{y}) = \prod_{i \in \{1,\dots,N_C\} \setminus \mathcal{I}_c} \mathcal{C}_i(\mathbf{y}) \tag{4.14}$$

and the corresponding convex cone $\mathcal{K}_{\mathcal{C}}^{\mathcal{I}_c}$.
This leads to a parametric family of optimization problems

$$P_1^{\mathcal{I}_c,\delta}: \quad \begin{cases} \min\limits_{\mathbf{u},\mathbf{y} \in \mathcal{U} \times \mathcal{Y}} \mathcal{J}^u(\mathbf{u},\mathbf{y}) + \mathcal{J}^{\mathcal{I}_c,\delta}(\mathbf{y}) \\ \text{subject to} \\ \qquad \mathcal{G}(\mathbf{u},\mathbf{y}) = 0_{\mathcal{Z}^\star}, \\ \qquad \mathcal{C}^{\mathcal{I}_c}(\mathbf{y}) \leq_{\mathcal{K}_{\mathcal{C}}^{\mathcal{I}_c}} 0, \\ \qquad u^e \in \mathcal{U}^{ad}. \end{cases} \tag{4.15}$$

with (partially) regularized state constraints. We denote the special case, in which $\mathcal{I}_{\mathcal{C}} = \{1,\dots,N_C\}$ (i.e. all state constraints have been regularized) by P_1^{δ}.
In the following sections we briefly cover the solvability of such optimization problems, followed by a description of a suitable optimization algorithm, and two application examples.

4.1 Existence of local minimizers with regularized state constraints

As discussed in the introduction of this chapter, one may not be able to prove the existence of a feasible point in many practical scenarios. Fortunately, we can at least guarantee the existence of a local minimum, if we can show that some inequality constraints can be satisfied, and relax (i.e. penalize or ignore) the remaining ones.
We start with the corner case, where we regularize all constraints, such that we have to solve an equality constrained optimization problem.

4.2 Proposition (Local solution of the equality constrained optimization problem)

Let $\mathcal{U}_{ad} \subset \mathcal{U}$ be a closed and convex, and $\mathcal{J}: \mathcal{U}_{ad} \times \mathcal{Y} \to \mathbb{R}$ be a continuous, and convex functional, which is bounded from below. Further, we assume that the operator $\mathcal{G}$ satisfies the assumptions of THEOREM *3.62. Then the fully regularized optimization problem P_1^{δ} specified in (4.15) has at least one local solution.*

Proof. Since $\mathcal{J}$ is bounded by assumption, we know that $J^\star := \inf_{\mathbf{u}} \mathcal{J}(\mathbf{u}, \mathcal{S}(\mathbf{u}))$ exists, and we can pick a minimizing sequence $\mathbf{u}_n \in \mathcal{U}_{ad}$. By THEOREM *3.62* we can pick a weakly convergent subsequence $\mathbf{u}_{n_k}$, such that $\mathbf{y}_{n_k} = \mathcal{S}(\mathbf{u}_{n_k})$ weakly converges to $\mathbf{y} \in \mathcal{Y}$. In particular, the weak limits satisfy $\mathbf{y} = \mathcal{S}(\mathbf{u})$ by the weak-weak*-continuity of $\mathcal{S}$.
Now we use that $\mathcal{J}$ is continuous and convex on $\mathcal{U}_{ad} \times \mathcal{Y}$, and therefore weakly lower semi-continuous. This yields

$$J^\star = \lim_{k\to\infty} \mathcal{J}(\mathbf{u}_{n_k}, \mathbf{y}_{n_k}) \geq \liminf_{k\to\infty} \mathcal{J}(\mathbf{u}_{n_k}, \mathbf{y}_{n_k}) \geq \mathcal{J}(\mathbf{u},\mathbf{y}) \tag{4.16}$$

such that $\mathcal{J}$ attains its local minimum $J^\star$ at $(\mathbf{u},\mathbf{y})$. □

Next, we consider the opposite scenario, where we can find an initial control $\mathbf{u}_0$, such that all constraints are strictly satisfied.

4.3 Corollary (Local solutions to the optimization problem)

Let $\mathcal{U}^{ad} \subset \mathcal{U}$ be a closed and convex, and $\mathcal{J} : \mathcal{U}^{ad} \times \mathcal{Y} \to \mathbb{R}$ be a continuous, and convex functional, which is bounded from below. Further, we assume that the operator $\mathcal{G}$ satisfies the assumptions of THEOREM *3.62. If we assume the existence of a control input $\mathbf{u}_0 \in \overset{\circ}{\mathcal{U}}_{ad}$ such that $\mathcal{G}(\mathbf{u}_0, \mathbf{y}_0) = 0$, and $\mathcal{C}(\mathbf{y}_0) \in \overset{\circ}{\mathcal{K}}_C$, then P_0 has local optimum $\mathbf{u}_0^\star$.*

Proof. By assumption, $\mathcal{C}$ is continuous. From $\mathcal{C}(\mathbf{y}_0) \in \overset{\circ}{\mathcal{K}}_C$ we conclude, that there is a number $\epsilon_y > 0$, such that

$$\mathcal{C}(\mathbf{y}) \in \overset{\circ}{\mathcal{K}}_C \qquad \forall \mathbf{y} \in B_{\epsilon_y}(\mathbf{y}_0). \tag{4.17}$$

By THEOREM *3.62*, the control-to-state operator $\mathcal{S}$ is continuous and bounded, such that there exists as second number $\delta_u > 0$, such that

$$\overset{\circ}{\mathcal{U}}_{ad} \supset B_{\delta_u}(\mathbf{u}_0) \ni \mathbf{u} \Rightarrow \mathbf{y} \in B_{\epsilon_y}(\mathbf{y}_0) \subset \overset{\circ}{\mathcal{Y}}_{ad} \tag{4.18}$$

and therefore $\mathcal{C}(\mathcal{S}(\mathbf{u})) \in \overset{\circ}{\mathcal{K}}_C$. We define the set $\mathcal{U}_{\delta_u} = \overline{B_{\delta_u}(\mathbf{u}_0) \cap \mathcal{U}_{ad}}$, which is a closed and convex subset of $\overset{\circ}{\mathcal{U}}_{ad}$. and formulate the reduced optimization problem without state inequality constraints

$$\min_{\mathbf{u},\mathbf{y}} \mathcal{J}(\mathbf{u}, \mathbf{y}) \text{ subject to } \mathcal{G}(\mathbf{u}, \mathbf{y}) = 0, \mathbf{u} \in \mathcal{U}_{\delta_u}, \mathbf{y} \in \mathcal{Y}_{ad} \tag{4.19}$$

which is locally equivalent to P_0. Finally, we apply PROPOSITION *4.2* to conclude the existence of a local minimum, which is attained at $(\mathbf{u}, \mathbf{y}) \in \mathcal{U}_{\delta_u} \times \mathcal{Y}_{ad}$. □

Now we combine both previous results, and immediately get the following result:

4.4 Corollary (Local solution for the partially regularized optimization problem)

Let $\mathcal{U}^{ad} \subset \mathcal{U}$ be a closed and convex, and $\mathcal{J} : \mathcal{U}^{ad} \times \mathcal{Y} \to \mathbb{R}$ be a continuous, convex, and bounded functional. Further, we assume that the operator $\mathcal{G}$ satisfies the assumptions of THEOREM *3.62. If we assume the existence of a control input $\mathbf{u}_0 \in \overset{\circ}{\mathcal{U}}^{ad}$ such that $\mathcal{G}(\mathbf{u}_0, \mathbf{y}_0) = 0$, and $\mathcal{C}^{\mathcal{I}_c}(()\mathbf{y}_0) \in \overset{\circ}{\mathcal{K}}_{\mathcal{C}}^{\mathcal{I}_c}$, then the optimization problem $P_1^{\mathcal{I}_c,\delta}$ has at least one local solution $\mathbf{u}_0^\star$ inside an open neighbourhood of $\mathbf{u}_0$*

Proof. Given $\mathcal{C}^{\mathcal{I}_c}(\mathbf{y}_0) \in \overset{\circ}{\mathcal{K}}_{\mathcal{C}}^{\mathcal{I}_c}$, and the continuity of $\mathcal{S}$ (which is ensured by THEOREM *3.62*), there exists an convex, open set $\mathcal{U}^{\mathcal{I}_c} \subset \mathcal{U}^{ad}$, such that $\mathbf{u}_0 \in \mathcal{U}^{\mathcal{I}_c}$.
Now we consider a modified version $\tilde{P}_1^{\mathcal{I}_c,\delta}$ of $P_1^{\mathcal{I}_c,\delta}$, where remove the remaining state constraints $\mathcal{C}^{\mathcal{I}_c}$, and replace the admissible set $\mathcal{U}^{ad}$ by $\mathcal{U}^{\mathcal{I}_c}$. Now we apply PROPOSITION *4.2*, which yields the desired result. □

4.2 Projected gradient descent in H^1

In CHAPTER 3 we have shown, that the residual formulation is continuously Fréchet differentiable. We are going to use this property in order to compute the gradient vector, which is going to build the basis of our first order optimization algorithm. For a broader discussion of optimization methods in Banach spaces, specifically projected gradient algorithms, we refer to [Hinze et al., 2009].
We consider the simplified optimization problem

$$\min_{\mathbf{u}\in\mathcal{U}} \mathcal{J}(\mathbf{u},\mathbf{y}) \tag{4.20}$$
$$\text{s.t. } \mathcal{G}(\mathbf{u},\mathbf{y}) = 0 \tag{4.21}$$
$$\mathbf{u} \in \mathcal{U}_{ad} \tag{4.22}$$

without (or only with regularized) state constraints.
If we presume, that our residual operator is sufficiently regular in a neighbourhood of its solutions, the operator

$$\mathbf{y}'(\mathbf{u}) = \mathcal{S}'(\mathbf{u}) = -\left(\mathfrak{D}_{\mathbf{y}}\mathcal{G}(\bar{\mathbf{u}},\bar{\mathbf{y}})\right)^{-1}\mathfrak{D}_{\mathbf{u}}\mathcal{G}(\bar{\mathbf{u}},\bar{\mathbf{y}}), \tag{4.23}$$

which is an element of $\mathrm{Lin}(\mathcal{U},\mathcal{Y})$, is well defined.
In the following, we presuppose that the below statement is true:

Assumption 4.5: Regularity assumption for $\mathcal{G}$ at solution points

The pair $(\bar{\mathbf{u}},\bar{\mathbf{y}}) \in \mathcal{U}\times\mathcal{Y}$ is a solution of the state equation $\mathcal{G}(\bar{\mathbf{u}},\bar{\mathbf{y}}) = 0$, such that $\mathcal{G}_{\mathbf{y}}(\bar{\mathbf{u}},\bar{\mathbf{y}})$ has a bounded inverse.

In view of (4.23), we define the *reduced cost functional*

$$f(\mathbf{u}) = \mathcal{J}(\mathbf{u},\mathcal{S}(\mathbf{u})) \tag{4.24}$$

whose derivative

$$\langle f'(\bar{\mathbf{u}}),\mathbf{d}\rangle_{\mathcal{U}^\star,\mathcal{U}} = \langle \mathfrak{D}_{\mathbf{u}}\mathcal{J}(\bar{\mathbf{u}},\mathcal{S}(\bar{\mathbf{u}})),\mathbf{d}\rangle_{\mathcal{U}^\star,\mathcal{U}} + \langle \mathfrak{D}_{\mathbf{y}}\mathcal{J}(\bar{\mathbf{u}},)\,\mathcal{S}'(\bar{\mathbf{u}}),\mathbf{d}\rangle_{\mathcal{U}^\star,\mathcal{U}} \tag{4.25}$$

at a point $\bar{\mathbf{u}}\in\mathcal{U}$ in direction $\mathbf{d}\in\mathcal{U}$ can be explicitly computed, if the derivative of the solution operator $\mathcal{S}$ is known. If one is only interested in the parts of $\mathbf{y}'$, which directly contribute to f', this approach probably inefficient. An alternative approach utilizes the adjoint of the linearized state equations

$$\mathcal{G}(\bar{\mathbf{u}},\bar{\mathbf{y}}) = 0_{\mathcal{Z}^\star}, \tag{4.26a}$$
$$\mathfrak{D}_{\mathbf{y}}\mathcal{G}(\bar{\mathbf{u}},\bar{\mathbf{y}})^\star\mathbf{z} = -\mathfrak{D}_{\mathbf{y}}\mathcal{J}(\bar{\mathbf{u}},\bar{\mathbf{y}}), \tag{4.26b}$$

which is well defined, if ASSUMPTION 4.5 holds true. This leads to an alternative representation

$$\langle f'(\bar{\mathbf{u}}),\mathbf{d}\rangle_{\mathcal{U}^\star,\mathcal{U}} = \langle \mathfrak{D}_{\mathbf{u}}\mathcal{J}(\bar{\mathbf{u}},\bar{\mathbf{y}}),\mathbf{d}\rangle_{\mathcal{U}^\star,\mathcal{U}} + \left\langle \left(\mathfrak{D}_{\mathbf{u}}\mathcal{G}(\bar{\mathbf{u}},\bar{\mathbf{y}})\right)^\star\mathbf{z},\mathbf{d}\right\rangle_{\mathcal{U}^\star,\mathcal{U}} \tag{4.27}$$

for the derivative of the reduced cost functional, which does not explicitly depend on $\mathbf{y}^\star$ any more. Using either approach, we can use the fast, that $\mathcal{U}$ is a Hilbert space, and apply the Riesz isomorphism $R:\mathcal{U}^\star\to\mathcal{U}$ to obtain a vector representative

$$\langle f'(\bar{\mathbf{u}}),\mathbf{d}\rangle_{\mathcal{U}^\star,\mathcal{U}} = (Rf'(\bar{\mathbf{u}}),\mathbf{d})_{\mathcal{U}} =: \left(\nabla_u^{\mathcal{U}} f(\bar{\mathbf{u}}),\mathbf{d}\right)_{\mathcal{U}} \tag{4.28}$$

of $f'(\bar{\mathbf{u}})$, which is called the *gradient* of f at $\bar{\mathbf{u}}$. The negative gradient is always a direction of descent, if the gradient is non-zero, such that we can expect the functional value to decrease, if we adjust $\bar{\mathbf{u}}$ in this direction.
Since we want to use this method to solve a non-linear optimization problem, we need to perform a line search to ensure, that the functional value actually decreases. The *projected Armijo rule*

$$f\left(\bar{\mathbf{u}}+\mathbf{d}\right)-f\left(\bar{\mathbf{u}}\right)\leq\gamma\left(\mathbf{d},\nabla_u^{\mathcal{U}}f(\bar{\mathbf{u}})\right)_{\mathcal{U}}=-\frac{\gamma}{\sigma}\left\|\sigma d\right\|_{\mathcal{U}}^2 \tag{4.29}$$

yields an appropriate termination rule for this line search procedure (see [Hinze et al., 2009]). Here, the *descent direction* is given by the scaled, negative gradient

$$\mathbf{d}=-\sigma\nabla_u^{\mathcal{U}}f(\bar{\mathbf{u}}), \tag{4.30}$$

with positive parameters σ and γ. Unless the magnitude of $\mathbf{d}$ is relatively small, and $\bar{\mathbf{u}}$ is sufficiently far away from the boundary of $\mathcal{U}^{ad}$, a step into the direction $\mathbf{d}$ is likely to result in an inadmissible control vector.
By its definition in CHAPTER 3 the admissible set $\mathcal{U}^{ad}$ is convex and closed within the Hilbert space $\mathcal{U}$, such that the *projection*

$$\hat{\mathbf{u}}=\mathbb{P}_{\mathcal{U}_{ad}}\left(\bar{\mathbf{u}}+\mathbf{d}\right):=\underset{\mathbf{u}\in\mathcal{U}_{ad}}{\arg\min}\,\frac{1}{2}\left\|\mathbf{u}-\bar{\mathbf{u}}-\mathbf{d}\right\|_{\mathcal{U}}^2 \tag{4.31}$$

is uniquely defined.
Combined, this results in the following optimization algorithm:

Algorithm 4.1: Projected gradient descent

0. Choose an initial control $\mathbf{u}^0\in\mathcal{U}_{ad}$, and a descent parameter $\gamma\in(0,1)$
for $k=0,1,\ldots$ **do**
   1. Compute $\mathbf{d}^k=-\nabla_u^{\mathcal{U}}f(\mathbf{u}^k)$
   2. Choose the largest $\sigma^k\in\left\{1,\frac{1}{2},\frac{1}{4},\ldots\right\}$ such that
      $f\left(\mathbb{P}_{\mathcal{U}_{ad}}\left(\mathbf{u}^k+\sigma^k\mathbf{d}^k\right)\right)-f\left(\mathbf{u}^k\right)\leq-\frac{\gamma}{\sigma^k}\left\|\mathbb{P}_{\mathcal{U}_{ad}}\left(\mathbf{u}^k+\sigma^k d^k\right)-\mathbf{u}^k\right\|_{\mathcal{U}}^2$
   3. Set $\mathbf{u}^{k+1}=\mathbb{P}_{\mathcal{U}_{ad}}\left(\mathbf{u}^k+\sigma^k d^k\right)$

   if $\left\|\mathbf{u}^{k+1}-\mathbf{u}^k\right\|_{\mathcal{U}}<\epsilon_{tol}$ **then**
      Stop and return $\mathbf{u}^{k+1}$

Next, we are going to take a closer look on the projection operator on the Hilbert space $H^1(I_t)$. For this purpose, we partition the squared H^1-distance

$$\frac{1}{2}\left\|u-\bar{u}+\sigma\nabla_u^H f(\bar{u})\right\|_{H^1(I_t)}^2=\underbrace{\frac{1}{2}\left(u,u\right)_{H^1(I_t)}}_{\mathfrak{a}(u,u)}+\underbrace{\left(u,\bar{u}\right)_{H^1(I_t)}-\left\langle\sigma f'(\bar{u}),u\right\rangle_{H^1(I_t)^\star,H^1(I_t)}}_{-\langle\phi,u\rangle_{H^1(I_t)^\star,H^1(I_t)}} \tag{4.32}$$

into an elliptic bilinear form $\mathfrak{a}$, and a linear functional remainder $\langle\phi,u\rangle$. Together with the affine constraint operator

$$\mathcal{C}(u)=\begin{pmatrix}u_{min}-u\\u-u_{max}\end{pmatrix} \tag{4.33}$$

with corresponding convex cone

$$\mathcal{K} = \left\{ u_1, u_2 \in H^1 \times H^1 \,|\, u_1, u_2 \geq 0 \right\}, \tag{4.34}$$

the orthogonal projection onto the admissible set

$$\mathcal{U}_{ad} := \{ \mathbf{u} \in \mathcal{U} \,|\, u_{min} \leq u \leq u_{max} \text{ a.e. in } I_t \} \tag{4.35}$$

is equivalent to the solution of the cone constrained optimization problem

$$\min_{u \in H^1(I_t)} \mathfrak{a}(u,u) - \langle \phi, u \rangle_{H^1(I_t)^\star, H^1(I_t)} \tag{4.36}$$

$$\text{s.t. } \mathcal{C}(u) \leq_{\mathcal{K}} 0 \tag{4.37}$$

in H^1.
This is an elliptic, bilateral obstacle problem with a continuous, coercive bilinear form $\mathfrak{a}$. In its discretized form, the optimality system

$$A\vec{u} - B^T \vec{\lambda} = \vec{\Phi} \tag{4.38}$$

$$\vec{\lambda} - \max\left\{ \vec{0}, \vec{\lambda} + c\left(\vec{\beta} - B\vec{u} \right) \right\} = 0 \tag{4.39}$$

of (4.36) can be efficiently solved by using an active set method. For implementation details, we refer to [Zhou et al., 2002], and [Kärkkäinen et al., 2003].
In the context of district heating networks, it is likely, that there is more than one boundary input which can be controlled.
We recall, that $\mathcal{U}$ was constructed as the Cartesian product

$$\mathcal{U} = \prod_{i=0}^{N_u} \mathcal{U}_i, \qquad \|\cdot\|_{\mathcal{U}}^2 = \sum_{i=0}^{N_u} \|\cdot\|_{\mathcal{U}_i}^2, \tag{4.40}$$

of finitely many Hilbert spaces (see DEFINITION *3.42*), whose norm (or scalar product) is given as the finite sum of norms (scalar products) for each control variable u_i. Therefore, we can split the projection problem into N_u sub-problems

$$\begin{array}{ll} \textbf{u}^\star \textbf{ is the solution of} & \forall i: \ \mathbf{u}_i^\star \textbf{ is the solution of} \\ \min_{\mathbf{u} \in \mathcal{U}} \frac{1}{2} \|\mathbf{u} - \bar{\mathbf{u}}\|_{\mathcal{U}}^2 & \iff \min_{\mathbf{u}_i \in \mathcal{U}_i} \frac{1}{2} \|\mathbf{u}_i - \bar{\mathbf{u}}_i\|_{\mathcal{U}_i}^2 \\ \text{s.t. } \mathcal{C}(\mathbf{u}) \leq_{\mathcal{K}} 0 & \text{s.t. } \mathcal{C}_i(\mathbf{u}_i) \leq_{\mathcal{K}_i} 0 \end{array}, \tag{4.41}$$

of which each fits exactly into the special case, which we described above.

4.3 Numerical discretization, sensitivities, and discrete adjoint

For the discretization of the advection operator we consider two different methods. The first one is a Runge-Kutta Discontinuous Galerkin (RKDG) scheme (see [Cockburn and Shu, 2001]) with upwind flux, and the implicit Euler (see e.g. [Quarteroni et al., 2007]) method for time integration. An alternative approach is given by a discretization of SECTION *3.1*, which results in a Euler-Lagrangian collocation method (see [Mohring et al., 2021]).
In both cases, the remaining algebraic equations are coupled implicitly with the advection sub-system, such that the evolution of the discretized state vector $\mathbf{y}_h^k$ at the time step t^k to the next one is given as the solution of a nonlinear system of equations

$$G\left(t^k, t^{k+1}; \mathbf{y}_h^k, \mathbf{y}_h^{k+1}, \mathbf{u}_h\right) =: G^k\left(\mathbf{y}_h^k, \mathbf{y}_h^{k+1}, \mathbf{u}_h\right). \tag{4.42}$$

Including an additional equation for the initial state, the complete discrete formulation of the model equations then takes the form

$$G^0\left(\mathbf{y}_h^0, \mathbf{u}_h\right) = 0, \tag{4.43a}$$
$$G^k\left(\mathbf{y}_h^k, \mathbf{y}_h^{k+1}, \mathbf{u}_h\right) = 0, \quad k = 1, \dots, N_t, \tag{4.43b}$$

which we commonly refer to by the term $G\left(\mathbf{y}_h, \mathbf{u}_h\right) = 0$, if we are not interested in one particular time step.
We are going to follow two different approaches for the computation of the gradient, which is then used within the algorithm presented in SECTION 4.2.

Given ASSUMPTION 4.5, an application of the implicit derivative rule (4.23) to the discretized system (4.43) yields the discrete *sensitivity equations*

$$S^k\left(\mathbf{u}_h\right) = D_{\mathbf{u}}\mathcal{S}'(\mathbf{u}_h) = -\left(D_{\mathbf{y}^k}G^k\right)^{-1}\left(D_{\mathbf{y}^{k-1}}G^k S^{k-1} + D_{\mathbf{u}}G^k\right). \tag{4.44}$$

We note, that this approach relies on the computability of several partial Jacobian matrices. An easy, robust, and efficient way to solve this problem numerically is given by *automatic differentiation*. We refer to [Griewank and Walther, 2008] for a general overview of this topic. Depending on the optimization problem we are trying to solve, this procedure might be inefficient, since it requires computing the sensitivities of all state variables at each given time.
Following the short discussion in the introduction of SECTION 4.2, we also consider the discrete counter part of the adjoint equation (4.26b), which results in a linear system of equations

$$D_{\mathbf{y}}G(\bar{\mathbf{u}}_h, \bar{\mathbf{y}}_h)^\star \mathbf{z}_h = -D_{\mathbf{y}}\mathcal{J}\left(\bar{\mathbf{u}}_h, \bar{\mathbf{y}}_h\right), \tag{4.45}$$

we assume that $G(\bar{\mathbf{u}}_h, \bar{\mathbf{y}}_h) = 0$.
By using the block structure of G shown in (4.43), we split up (4.45), and obtain a linear time stepping scheme

$$D_{\mathbf{y}^k}G^k(\mathbf{y}_h^{k-1}, \mathbf{y}_h^k, \mathbf{u}_h)^\star z_h^k = -D_{\mathbf{y}_h^k}\mathcal{J}\left(\mathbf{y}_h, \mathbf{u}_h\right), \quad k = N_t, \tag{4.46a}$$
$$D_{\mathbf{y}^k}G^k(\mathbf{y}_h^{k-1}, \mathbf{y}_h^k, \mathbf{u}_h)^\star z_h^k + D_{\mathbf{y}^k}G^{k+1}(\mathbf{y}_h^k, \mathbf{y}_h^{k+1}, \mathbf{u}_h)^\star z_h^k = -D_{\mathbf{y}_h^k}\mathcal{J}\left(\mathbf{y}_h, \mathbf{u}_h\right), \quad k = N_t - 1, \dots, 1, \tag{4.46b}$$
$$D_{\mathbf{y}^0}G^0(\mathbf{y}_h^0, \mathbf{u}_h)^\star z_h^0 + D_{\mathbf{y}^0}G^1(\mathbf{y}_h^0, \mathbf{y}_h^1, \mathbf{u}_h)^\star z_h^0 = -D_{\mathbf{y}_h^k}\mathcal{J}\left(\mathbf{y}_h, \mathbf{u}_h\right), \tag{4.46c}$$

which moves backwards in time and whose solution is the discrete adjoint state $\mathbf{z}_h$.

4.4 Application of the H^1 projected gradient algorithm to a single pipeline network

For our first model example, we consider the single-consumer-single-producer network introduced in SECTION 3.1 without reaction term and hydraulic equations, which has been partially published in [Linn et al., 2021]. Following the general optimization model, which we introduced at the beginning of this chapter, this leads to the following optimization prob-

lem:

$$\min_{u\in\mathcal{U}} \frac{\alpha_0}{2}\int_{I_t} u^e(t)^2\,dt + \frac{\alpha_1}{2}\int_{I_t}\left(\partial_t u^e(t)\right)^2\,dt \tag{4.47a}$$

subject to

$$\partial_t e + v\partial_x e = 0 \tag{4.47b}$$
$$e(\cdot,0) = u^e \tag{4.47c}$$
$$v(e(\cdot,L) - e^{ret}) = g \tag{4.47d}$$
$$e(t_0) = e_{init} \tag{4.47e}$$
$$v(t_0)\partial_x(e_{init}) = 0 \tag{4.47f}$$
$$e_{init} = u^e(t_0) \tag{4.47g}$$
$$u^e_{min} \le u^e \le u^e_{max} \tag{4.47h}$$
$$v(u^e - e^{ret}) \le \Delta Q_{max}. \tag{4.47i}$$

Here, we have eliminated all flux variables, such that the power constraint of the producer is turned into the mixed formulation (4.47i). The two additional equations (4.47f) and (4.47g) connect the (spatially constant) initial state to the initial value $u^e(t_0)$ of the control variable. Our goal is to derive the adjoint form of the linearized system, and apply ALGORITHM *4.1* which was outlined in the previous section. Since we cannot be sure that the mixed constraint is feasible, we choose to regularize it by adding a Moreau-Yosida penalty term. This leads to the following modified optimization problem

$$\min_{u\in\mathcal{U}} \frac{\alpha_0}{2}\int_{I_t} u^e(t)^2\,dt + \frac{\alpha_1}{2}\int_{I_t}\left(\partial_t u^e(t)\right)^2\,dt + \frac{\delta}{2}\int_{I_t}\left(\left(v(t)(u^e(t)-e^{ret}) - \Delta Q^{max}\right)^+\right)^2 \tag{4.48a}$$

subject to

$$\partial_t e + v\partial_x e = 0 \tag{4.48b}$$
$$e_{in} = u^e \tag{4.48c}$$
$$v(e_{out} - e^{ret}) = g \tag{4.48d}$$
$$e(t_0) = e_{init} \tag{4.48e}$$
$$v(t_0)\partial_x(e_{init}) = 0 \tag{4.48f}$$
$$e_{init} = u^e(t_0) \tag{4.48g}$$
$$u^e_{min} \le u^e \le u^e_{max}, \tag{4.48h}$$

which introduces an additional *penalty parameter* δ.
Now we utilize the structure of the linearized system, which we already derived in SECTION *3.3.4*, and apply the partial integration rule for Gelfand triples to obtain

$$\partial_t z^{adv} + \bar{v}\partial_x z^{adv} = 0 \tag{4.49a}$$
$$\int_\Omega z^{adv}(t)\partial_x\bar{e}(t)\,dx = z^{adv}(t,L)\left(\bar{e}(t,L) - e^{ret}\right) + \delta\left(\bar{u^e} - e^{ret}\right)\left(\bar{v}\left(\bar{u^e} - e^{ret} - \Delta Q^{max}\right)\right)^+ \tag{4.49b}$$
$$z^{adv}(t_f) = 0 \tag{4.49c}$$

where have already eliminated all remaining adjoint states ($z^{e:in}$, $z^{consumer}$, etc.) due to the simple boundary conditions. The Fréchet derivative of the reduced cost functional can

now be represented as

$$\langle f'(\bar{u^e}), u^e - \bar{u^e} \rangle_{\mathcal{U}^\star, \mathcal{U}} = \alpha_0 \left(\bar{u^e}, u^e - \bar{u^e}\right)_{L^2(I_t)} + \alpha_1 \left(\partial_t \bar{u^e}, \partial_t \left(u^e - \bar{u^e}\right)\right)_{L^2(I_t)} \tag{4.50}$$

$$+ \left(u^e(t_0) - \bar{u^e}(t_0)\right) \int_\Omega z^{adv}(t_0)(x)\, dx \tag{4.51}$$

such that we can compute its H^1 representative via the Riesz isomorphism, and apply ALGORITHM *4.1*.

In order to test this optimization algorithm, we selected a reference pipeline with length $L = 1000m$, together with a normalized, periodic consumer, shown in the lower graph in FIGURE *4.1*, with two local maxima of different magnitude per period. The forward and adjoint equations using a first order discontinuous Galerkin scheme with BDF-1 time stepping, with $\Delta x = 1m$, and $\Delta t = 60s$. The simulation time interval I_t covers a time span of 3 days, such that effects caused by the spatially constant initial state have enough time to decay, and a periodic system state can be reached.

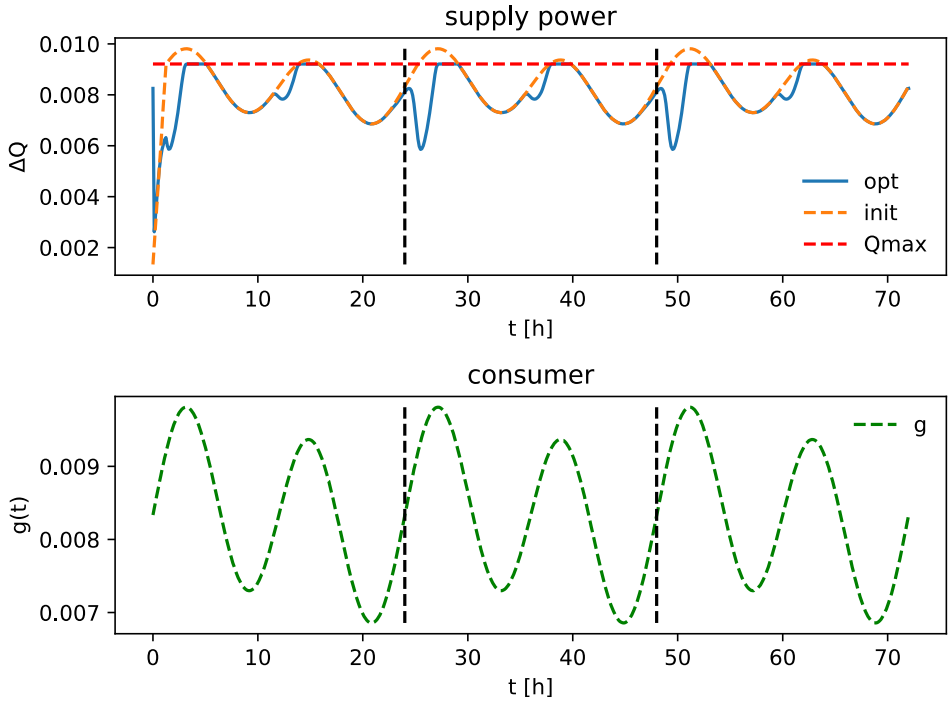

Figure 4.1: *Upper graph*: comparison between the producer's normalized supply power for the initial and optimized control. *Lower graph*: normalized consumer demand

FIGURE *4.2* and the upper graph in FIGURE *4.1* show, that effects of the initial state can still be observed during the first day, but vanish during the two subsequent ones, as desired.

The effects of the optimized control can be clearly recognized: While the initial control causes an overshooting of the supply power at local maxima of the consumer demand g, the optimized control manages to cut off the undesired peak values, such that the power constraint (4.47i) is satisfied.

This is achieved by pre-heating the network ahead of demand peaks, as shown in FIGURE *4.2*. The simple example demonstrates, that the model problem is already able to reproduce

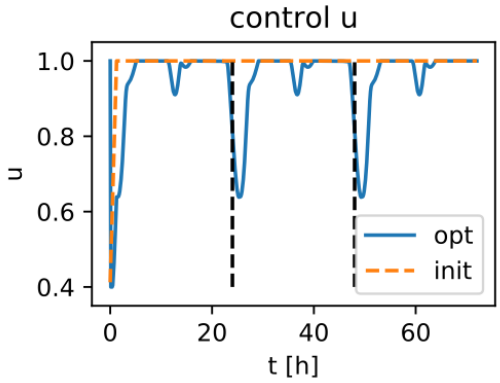

Figure 4.2: Initial and optimized normalized control input

some of the effects, which are encountered in more complex, real world district heating networks, as discussed in the subsequent SECTION *4.5*.

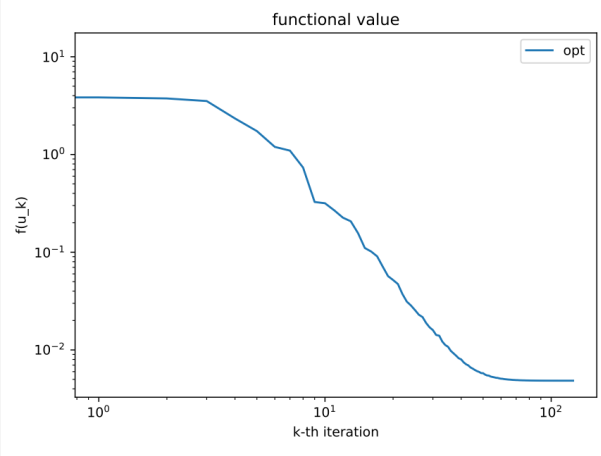

Figure 4.3: Value of the cost functional throughout the iterations of the PGD algorithm

However, the performance characteristics of the PGD algorithm, as plotted in FIGURE *4.3*, reveal that a large amount of iterations is needed until stationarity is reached.

4.5 Optimal operation of a real world network using discrete sensitivity propagation

After the simple example covering a model problem for a single pipeline, we demonstrate the solvability of such power constrained optimization problems for a real world network, whose topology is shown in FIGURE *4.4*. Unlike the class of models analysed in CHAPTER *3*, this network contains loops, such that we have to adapt the inflow boundary conditions according to REMARK *2.8*. Furthermore, we note that the existence of loops can lead to *contact discontinuities*. In order to see this, imagine the following scenario: We observer 3-way junction with two inflowing pipelines - one containing hot, the other one containing cold water. The resulting mixing temperature of the out-flowing pipe lies somewhere in between. If the flow direction of one inflowing and the outflowing pipe change, the former inflowing one is exposed to a boundary value which does not continuously match its internal temperature distribution. For a more elaborate example we refer to [Mohring et al., 2021]. This detail is important for the development of high resolution schemes, but negligible four our use case, where the coarse discretization leads to a high numerical diffusion. The methodology and results presented in this section have been partially published in [Linn et al., 2019] and [Mohring et al., 2021].

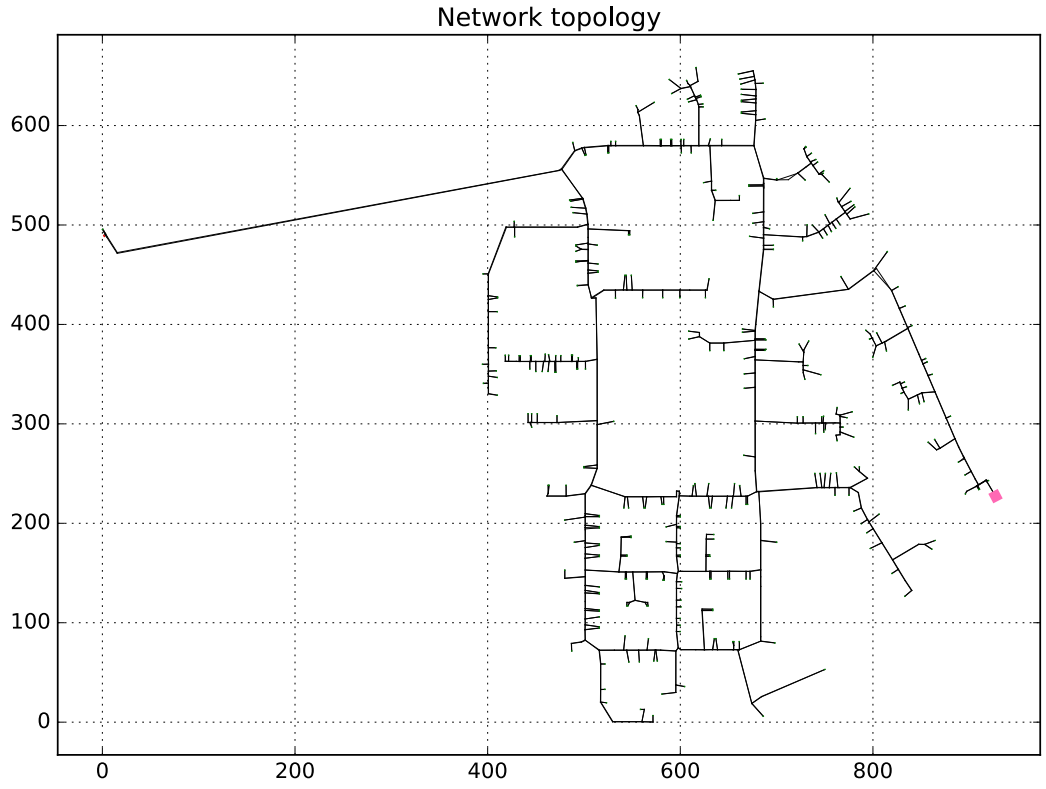

Figure 4.4: Topology of a real district heating network, provided by Technische Werke Ludwigshafen am Rhein AG (TWL)

For this example, we consider the following optimization problem

$$\min_{u^e \in \mathcal{U}^e} \alpha \int_{I_t^{day}} u^e(t)^2 \, dt + \int_{I_t^{day}} \left(\partial_t u^e(t)\right)^2 \, dt =: \mathcal{J}\left(u^e\right) \tag{4.52a}$$

subject to

$$\mathcal{G}(\mathbf{u}, \mathbf{y}) = 0 \tag{4.52b}$$

$$e_{i(c)} \leq e^{min} \qquad \forall c \in \mathcal{A}_C \tag{4.52c}$$

$$Q_{s:in} + Q_{s:out} \leq \Delta Q^{max} \tag{4.52d}$$

$$u^e(t_0) = u^e(t_f) \tag{4.52e}$$

$$u^{e,min} \leq u^e \leq u^{e,max} \tag{4.52f}$$

which aims to find the most regular solution (in terms of the H^1 semi-norm), such that all state constraints are satisfied. To avoid undesired transient effects in the starting phase caused by an unfavourable initial state, the control input is a priori set to be periodic with a period length of a day. The hydraulic control inputs u^{p_0} and $u^{\Delta p}$ are prescribed in advance, and are treated as boundary conditions.
The basis of our optimization approach for this problem is the discretized version of (4.52)

$$\min_{u_h^e \in \mathcal{U}_h^e} \alpha \int_{I_t^{day}} u_h^e(t)^2 \, dt + \int_{I_t^{day}} \left(\partial_t u_h^e(t)\right)^2 \, dt =: \mathcal{J}\left(u_h^e\right) \tag{4.53a}$$

subject to

$$G\left(\mathbf{u}_h, \mathbf{y}_h\right) = 0 \tag{4.53b}$$

$$C\left(\mathbf{y}_h\right) \leq 0 \tag{4.53c}$$

$$u_h^e(t_0) = u_h^e(t_f) \tag{4.53d}$$

$$u^{e,min} \leq u_h^e \leq u^{e,max} \tag{4.53e}$$

where the state constraints are collected in the operator C, whose construction was described in the beginning of this chapter. Given a solution $\mathbf{y}_h$ of the discrete state equations, we now apply the discrete sensitivity propagation formula (4.44) to derive a first order approximation

$$C\left(\mathbf{u}_h + \mathbf{d}_h\right) = C\left(\mathbf{u}_h\right) + \underbrace{\left(\sum_{k=0}^{N_t} D_{\mathbf{y}^k} C\left(\mathbf{y}_h\right) S^k\right)}_{\tilde{C}(\mathbf{y}_h, \mathbf{u}_h)} \mathbf{d}_h + \mathcal{O}\left(\left\|\mathbf{d}_h\right\|^2\right) \tag{4.54}$$

of the constraint mapping C, which considers changes $\mathbf{u}_h$ in direction $\mathbf{d}_h$. This leads to the *reduced optimization model*

$$\min_{\mathbf{d}_h \in \mathcal{U}_h^e} \frac{1}{2} \mathcal{H}\left(\mathbf{d}_h, \mathbf{d}_h\right) \tag{4.55a}$$

subject to

$$C\left(\mathbf{u}_h\right) + D\left(\mathbf{u}_h\right) \cdot \mathbf{d}_h \leq 0 \tag{4.55b}$$

$$u^{e,min} \leq \mathbf{u}_h + \mathbf{d}_h \leq u^{e,max} \tag{4.55c}$$

$$\mathbf{d}_h(t_0) = \mathbf{d}_h(t_f) \tag{4.55d}$$

$$\left\|\mathbf{d_h}\right\|_{max} \leq M \tag{4.55e}$$

which does not depend on the state vector $\mathbf{y}_h$ any more. The new objective functional

$$\mathcal{H}\left(\mathbf{d}_h, \mathbf{d}_h\right) := 2\alpha \int_{I_t^{day}} \mathbf{d}_h(t)^2 \, dt + 2 \int_{I_t^{day}} \left(\partial_t \mathbf{d}_h(t)\right)^2 \, dt \tag{4.56}$$

is the second Fréchet derivative of $\mathcal{J}$, evaluated with $\mathbf{d}_h$ in both arguments. This is a strictly convex optimization problem with linear constraints. For its solution, we use the algorithm presented in [Goldfarb and Idnani, 1983]. The solution of the reduced optimization problem (4.55) yields a direction of descent required in the following algorithm:

Algorithm 4.2: Sequential linear-quadratic optimization

Choose an admissible initial control $\mathbf{u}_h^{\langle 0\rangle}$ such that $u^{e,min} \leq \mathbf{u}_h^{\langle 0\rangle} \leq u^{e,max}$
for *l=0,1,...* **do**
  Solve the forward system for $\mathbf{u}_h^{\langle l\rangle}$ and simultenously compute the sensitivity matrices $S^{\langle l\rangle,(k)}$
  Set up the reducied linear-quadratic problem (4.55) and solve it to obtain $\mathbf{d}_h^{\langle l\rangle}$
  if $\left\|\mathbf{d}_h^{\langle l\rangle}\right\| < \epsilon^{tol}$ **then**
    return $\mathbf{u}^{\langle l\rangle}$
  else
    Set $\mathbf{u}_h^{\langle l+1\rangle} = \mathbf{u}_h^{\langle l\rangle} + \mathbf{d}_h^{\langle l\rangle}$ and proceed with the next iteration, or abort if $l = l^{max}$.

We apply ALGORITHM *4.2* to solve (4.52) in an optimal control scenario for the network shown in FIGURE *4.4* (see [Linn et al., 2019], and [Mohring et al., 2021]). The optimization interval I_t covers a time span of a whole week. The consumers have been modelled according to the standardized consumption profiles [BGW, 2006], which we already have covered in SECTION *2.4*, where the profile of a reference day is continued periodically to the whole time interval. In a initialization step, we reset the initial state $\mathbf{y}_h(t_0)$ to a periodic solution of the system, obtained for a constant control input with value $u_h^e(t_0)$ at the beginning of each iteration of ALGORITHM *4.2*.

A local optimal solution to this problem is shown in FIGURE *4.5*. We can observe, that the power peaks have been avoided as desired. This is achieved by raising the temperature supplied to the forward flow networks in advance of the expected increase of consumer demands.

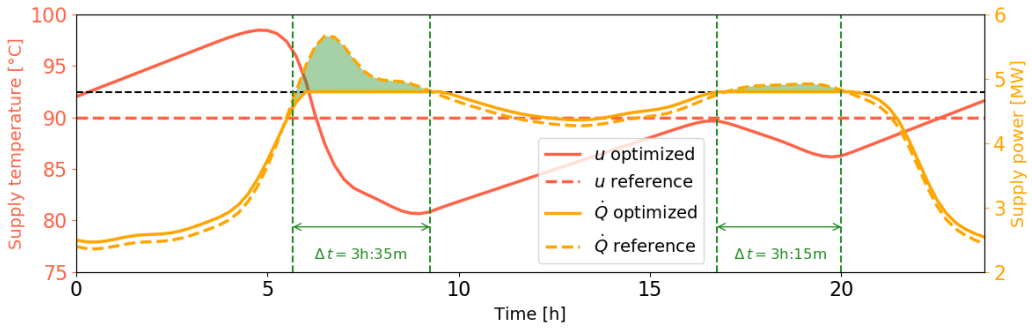

Figure 4.5: Supply temperature $T(u^e)$ and supply power ΔQ for the reference and optimized control input [Linn et al., 2019]

This is a common effect in district heating networks, which we were able to replicate with our simplified model problem discussed in SECTION *4.4*.

FIGURE 4.6 displays the net mass flux of the system corresponding to the supply temperature and supply power depicted FIGURE 4.5.

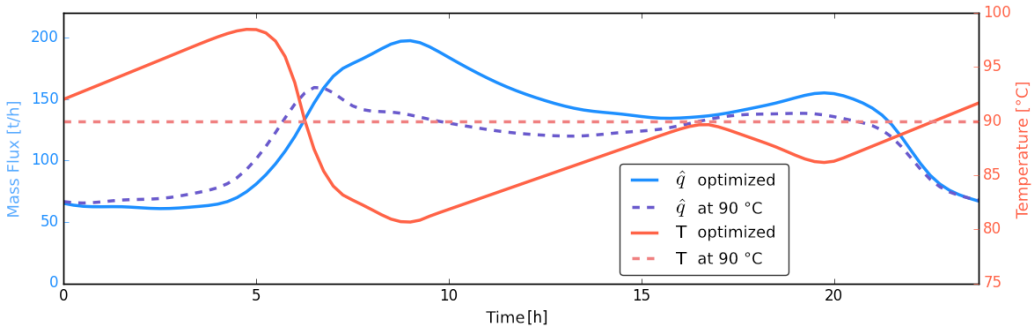

Figure 4.6: Supply temperature $T(u^e)$ and producer mass flow $\hat{q}$ for the reference and optimized control input

This second example demonstrates that our algorithm is able to handle optimal control problems for real world district heating networks at a larger scale. With these remarks, we conclude the discussion of application examples for the theoretical framework presented in CHAPTER 3.

Chapter 5

Summary, conclusion & outlook

In our thesis we have dealt with mathematical modelling and simulation of district heating networks (DHN).

The pipeline model set up in CHAPTER 2 accounts for fluid flow and energy transport. It is based on the Euler equations, includes a physical model of the relevant thermodynamic properties of water, and can be assembled to a DHN model by making use of conservation laws and some elementary modelling considerations from the engineering context. Our model provides an adaption and extension of existing mathematical models as presented in [Krug et al., 2019] or [Mohring et al., 2021] w.r.t. thermodynamically consistent water modelling, and the solvability of the model equations independent of the feasibility of state inequality constraints.

The results of our detailed mathematical analysis presented in CHAPTER 3 comprise a solution approach of the advection problem using the method of characteristics, with known order of wave propagation. We also provided a generalization to C^0 and H^1 data, along with a weak residual formulation in Bochner spaces, which is differentiable and has better continuity properties compared to other existing approaches. Our weak formulation in Bochner spaces is motivated by the solution theory for parabolic equations and permits differentiability and weak-weak* continuity. The first property is necessary to establish optimality conditions for this non-convex system, the second one aids as a theoretical tool to prove existence of local minimizers.

The two case studies presented in CHAPTER 4 indicate how the theoretical results of CHAPTER 3 can be favourably utilized to perform transient simulations of real world DHN and optimize their performance by optimal control.

In our first example we demonstrated the application of the H^1 projected gradient algorithm to a single pipeline network. In our second example we address the problem of an optimal operation of a real world network using discrete sensitivity propagation. Due to the large number of state constraints penalty regularization becomes a numerically ill conditioned procedure. In our numerical approach, we use the sensitivities to linearize the state constraints, and then solve a sequence of linearized optimization problems. The examples indicate that the theoretical results of CHAPTER 3 can be favourably utilized to perform transient simulations of real world DHN and optimize their performance by optimal control.

The theoretical framework developed within this thesis is restricted to networks without loops and flow indirections. While DHN fitting in this category make up a considerable amount of industrial use cases, more complicated network topologies containing loops occur in practice likewise frequently. Therefore, it would be desirable to extend the theory to such cases as well. A viable approach in this direction would be an asymptotic regularization of the advection equation by adding artificial viscosity terms, for example by

applying an operator splitting approach similar to the one used in the development of local discontinuous Galerkin methods (see [Cockburn and Shu, 1998]).
As we have seen in the mathematical analysis of our network model, the hydraulic component is tightly coupled to the consumers' predicted consumption. While it is reasonable to assume, that a consumer's actual consumption behaviour is relatively close to our prediction model based on historical data, we have to accept that some aspects of each consumer's behaviour cannot be modelled with in a fully deterministic sense. This motivates an extension of the consumer model to a probabilistic one. Interesting follow up questions include extending the theoretical model to the domain of stochastic calculus, investigating possibilities of performing uncertainty quantification and solving stochastic robust optimization problems for district heating networks.
As far as the implementation of a feasible optimization algorithm is concerned, we have only been able to real world use cases using a discretize first approach, whereas the optimize first alternative has only been applied to the single pipeline model. Due to the typically increasing number of inequality state constraints with increasing network size, it would be of interest to investigate appropriate constraint regularization methods for large scale networks.

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Academic curriculum vitae

Dominik Linn

05/2018 - 11/2022	PhD studies TU Kaiserslautern Fraunhofer Institute for Industrial Mathematics Kaiserslautern
05/2016 - 04/2018	Scientific employee Fraunhofer Institute for Industrial Mathematics Kaiserslautern
10/2012 - 04/2016	Master of Science in Industrial Mathematics (minor: Physics) TU Kaiserslautern
08/2012 - 06/2013	Erasmus student exchange Chalmers Technical University Göteborg, Sweden
10/2009 - 09/2012	Bachelor of Science in Mathematics (minor: Physics) TU Kaiserslautern
07/2008 - 03/2009	Civil service
03/2008	Abitur Albert-Schweitzer-Gymnasium Kaiserslautern

Akademischer Lebenslauf

Dominik Linn

05/2018 - 11/2022	Promotion TU Kaiserslautern Fraunhofer ITWM Kaiserslautern
05/2016 - 04/2018	Wissenschaftlicher Mitarbeiter Fraunhofer ITWM Kaiserslautern
10/2012 - 04/2016	Master of Science in Technomathematik (mit Nebenfach Physik) TU Kaiserslautern
08/2012 - 06/2013	Erasmus Austauschprogramm Chalmers TU Göteborg, Schweden
10/2009 - 09/2012	Bachelor of Science in Mathematik (mit Nebenfach Physik) TU Kaiserslautern
07/2008 - 03/2009	Zivildienst
03/2008	Abitur Albert-Schweitzer-Gymnasium Kaiserslautern