Feasibility for Maximal Uncertainty Sets in Robust Optimization with Application to Gas Networks

Zulässigkeit für maximale Unsicherheitsmengen in robuster Optimierung mit Anwendung in Gasnetzen

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Zusammenfassung

Zulässigkeit für maximale Unsicherheitsmengen in robuster Optimierung mit Anwendung in Gasnetzen

Viele Entscheidungen im realen Leben basieren aus unterschiedlichen Gründen auf unsicheren Daten. Eine mögliche Quelle für Unsicherheiten können Abweichungen in Vorhersagen und Prognosen, beispielsweise für den zukünftigen Bedarf von Wasserstoff, sein. Unsicherheiten in den Daten führen zu unsicheren Parametern in Optimierungsproblemen, die häufig reale Entscheidungsprozesse unterstützen. Die Berücksichtigung von Unsicherheiten in Optimierungsproblemen ist von großer Bedeutung, da bereits kleine Störungen in den Daten zu suboptimalen oder sogar unzulässigen Lösungen führen können. In dieser kumulativen Dissertation fokussieren wir uns auf den etablierten Ansatz der robusten Optimierung, um Unsicherheiten in Optimierungsproblemen zu berücksichtigen. Das Hauptziel der robusten Optimierung ist die Berechnung einer Lösung, die zulässig ist für alle – gewöhnlich unendlich viele – Unsicherheiten innerhalb einer vorgegebenen Unsicherheitsmenge und optimal unter dieser Bedingung ist. Ein Großteil der Literatur behandelt die Berechnung einer solchen robusten Lösung. Die Wahl der gegebenen Unsicherheitsmenge ist vergleichsweise wenig untersucht. Häufig wird die Wahl der Unsicherheitsmenge durch anwendungsorientierte Aspekte bestimmt. Dennoch ist es im Allgemeinen nicht zu erwarten, dass die exakte „Größe“ der Unsicherheitsmenge vor dem Optimierungsprozess bekannt ist. Zu groß gewählte Unsicherheitsmengen können zu unzulässigen robusten Optimierungsproblemen führen. Um robuste Unzulässigkeit auf Grund der Wahl der Unsicherheitsmenge zu vermeiden, ist es hilfreich, die maximale „Größe“ einer gegebenen Unsicherheitsmenge zu kennen, sodass mindestens eine robuste Lösung existiert. In dieser kumulativen Dissertation untersuchen wir maximale Unsicherheitsmengen, die Zulässigkeit für robuste Optimierungsprobleme garantieren, sowohl für gemischt-ganzzahlige lineare Probleme als auch im Kontext von Gasnetzen.

Im ersten Teil dieser kumulativen Dissertation fassen wir unsere erzielten Ergebnisse bezüglich maximaler Unsicherheitsmengen mit Zulässigkeitsgarantie zusammen und diskutieren die Resultate. Der zweite Teil beinhaltet die reproduzierten Publikationen und Vorveröffentlichungen, die alle Details zu unseren vorgestellten Ergebnissen enthalten. Die jeweiligen Beiträge des Autors dieser kumulativen Dissertation zu diesen Artikeln sind im Abschnitt „Author’s Contributions“ ab Seite ix dargelegt. Nachfolgend beschreiben wir kurz den Inhalt des ersten Teils der Dissertation.

Für gemischt-ganzzahlige lineare Optimierungsprobleme betrachten wir ein bestimmtes Maß für die Größe der Unsicherheitsmenge: „den Radius der robusten

Zulässigkeit/radius of robust feasibility“ (RRF). Wir führen den RRF für gemischt-ganzzahlige lineare Optimierungsprobleme ein und analysieren den RRF eines gemischt-ganzzahligen linearen Problems und seiner kontinuierlichen Relaxierung unter den üblichen Annahmen der Literatur. Anschließend erweitern wir den RRF um „sichere“ Variablen und Nebenbedingungen, das heißt Variablen und Nebenbedingungen, die nicht von Unsicherheiten betroffen sind. Wir entwickeln Lösungsmethoden, die den RRF mit sicheren Variablen und Nebenbedingungen berechnen, und wenden diese in einer ausführlichen numerischen Studie an. Mit Hilfe unserer Ergebnisse können wir den „Preis der Robustheit“ durch Adjustieren der Größe der Unsicherheitsmenge kontrollieren.

Zusätzlich untersuchen wir die zweistufigen robusten Probleme der Buchungsvalidierung und der Berechnung von maximalen technischen Kapazitäten im europäischen Entry-Exit Gasmarktsystem. Eine Buchung ist ein Vertrag zwischen Gashändlern und dem Fernleitungsnetzbetreiber (FNB) bezüglich Ein- und Ausspeisekapazitäten im Gasnetz. Hierbei garantiert der FNB, dass jeder balancierte Lastfluss innerhalb der Buchung im Netz transportiert werden kann. Technische Kapazitäten sind Knotenkapazitäten, die die Buchungen begrenzen und somit maximal buchbare Kapazitäten ausweisen. Bis auf technische Feinheiten entsprechen die Buchungsvalidierung und die Berechnung maximaler technischer Kapazitäten der Entscheidung über Zulässigkeit beziehungsweise dem Lösen eines spezifischen zweistufigen robusten nichtlinearen Optimierungsproblems. Das Hauptziel dieses robusten Problems besteht in der Berechnung einer maximalen Unsicherheitsmenge von balancierten Lastflüssen, sodass jeder dieser Lastflüsse im Netz transportiert werden kann. Wir untersuchen das betrachtete zweistufige robuste Optimierungsproblem algorithmisch mit Fokus auf nichtlinearen Modellierungen des Gastransports. Dabei betrachten wir passive Netze, die nur aus Rohren bestehen, und aktive Netze, die zusätzlich aktiv steuerbare Kompressoren und Regler enthalten. Wir analysieren strukturelle Eigenschaften, beispielsweise (Nicht-)Konvexität, der Menge der zulässigen Buchungen als auch der Menge der zulässigen balancierten Lastflüsse für verschiedene Modellierungen des Gasflusses. Aus der Literatur ist bekannt, dass die Zulässigkeit einer Buchung in polynomieller Zeit für passive Netze mit Baumstruktur entschieden werden kann. Dieses Resultat kann auch mit Hilfe unserer Ergebnisse, basierend auf einer leicht unterschiedlichen Herangehensweise, gezeigt werden. Wir entwickeln einen Algorithmus, der die Zulässigkeit einer Buchung für passive Netze bestehend aus einem Kreis in polynomieller Zeit entscheidet. Die Buchungsvalidierung auf allgemeinen passiven Netzen ist coNP-schwer. Zusätzlich charakterisieren wir zulässige Buchungen für Netze mit Kompressoren und Reglern. Basierend auf den Ergebnissen für Buchungen erzielen wir Resultate zur Berechnung maximaler technischer Kapazitäten in passiven Netzen mit Baumstruktur. Diese Ergebnisse ermöglichen es, ein mehrstufiges Modell des europäischen Entry-Exit Gasmarktes aus der Literatur für passive Netze mit Baumstruktur in realer Größe und einem nichtlinearen Modell für den Gastransport zu lösen. Abschließend weisen wir darauf hin, dass unsere Ergebnisse auch zu anderen potenzialbasierten Netzwerkproblemen beitragen können, wie zum Beispiel der Berechnung einer robusten Durchmesserauswahl für baumförmige Wasserstoffnetze mit Bedarfsunsicherheiten.

Abstract

Robust optimization is a popular approach to protect an optimization problem against uncertain data within a user-specified set of scenarios, the so-called uncertainty set. In many cases, the choice of the uncertainty set is driven by the application. In general, it can be elusive to assume that the exact "size" of the uncertainty set can be specified prior to the optimization process. Overly large sized uncertainty sets can lead to infeasible robust optimization problems. To avoid robust infeasibility due to the choice of the uncertainty set, it is useful to know the maximal "size" of a given uncertainty set such that feasibility of the robust optimization problem is still guaranteed. We study maximal uncertainty sets that guarantee robust feasibility for general mixed-integer linear problems (MIPs) and in the context of gas networks in this cumulative dissertation.

In the first part, we summarize and discuss our results developed over the last years. The second part of this cumulative dissertation contains reprints of our original articles and preprints, which contain all details of the presented results. We also refer to these articles throughout the first part of this dissertation.

For general MIPs, we consider a specific notion for the maximal size of a given uncertainty set: the radius of robust feasibility (RRF). We introduce and study the RRF for MIPs under common assumptions from the literature and then extend the RRF to include "safe" variables and constraint, i.e., variables and constraints that are not affected by uncertainties. We further develop methods for computing the RRF of linear and mixed-integer linear problems with safe variables and constraints and successfully apply them to instances of the MIPLIB 2017 library. Based on our results, we can control the price of robustness by adjusting the size of the uncertainty set.

Moreover, we study the two-stage robust problems of deciding the feasibility of a booking as well as of computing maximal technical capacities within the European entry-exit gas market system. A booking is a capacity-right contract for which the transmission system operator has to guarantee that every balanced load flow below the booking can be transported through the network. Maximal technical capacities bound these bookings and, thus, describe maximal bookable capacities. Except for some technical subtleties, these robust problems lead to deciding the feasibility as well as solving a specific two-stage robust nonlinear optimization problem. The main goal of this problem consists of computing a maximal uncertainty set of balanced load flows so that for each of these load flows there is a feasible transport through the network. We study this problem algorithmically with focus on nonlinear models of gas transport. We analyze structural properties such as (non-)convexity of the set of feasible bookings and of the set of feasible balanced load flows for different models of gas transport. For deciding the feasibility of a booking, we develop a polynomial-time algorithm for single-cycle networks consisting of pipes. We also characterize feasible bookings in networks with compressors and control valves. Based on the results for bookings, we provide results for computing maximal technical capacities in tree-shaped networks. We note that our results can also contribute to other potential-based network problems such as computing a robust diameter selection for tree-shaped hydrogen networks with demand uncertainties.

Author's Contribution

This dissertation is based on several peer-reviewed journal articles that are published or accepted for publication and additionally includes submitted articles that are currently under review or in revision. The dissertation is split into Part A and Part B. We provide an extended summary regarding the corresponding articles in Part A. This summary contains the main ideas and the scientific contributions of these articles as well as illustrates their interrelationships. Part B consists of the reprints of the corresponding publications and preprints. In the following, we disclose the author's contribution to each article. We note that except for articles [JT5] and [JT6] the authors are given in alphabetical order.

[JT1] F. Liers, L. Schewe, and J. Thürauf. "Radius of Robust Feasibility for Mixed-Integer Problems". In: *INFORMS Journal on Computing* (2021). Published online. DOI: 10.1287/ijoc.2020.1030

The general idea to research the radius of robust feasibility for mixed-integer problems was proposed by Frauke Liers and Lars Schewe in joint discussions with Johannes Thürauf. The theoretical results and algorithms were developed by Johannes Thürauf under supervision of the other authors. He further was responsible for the corresponding implementation and conducted the computational study in joint discussion with the other authors. He also primarily wrote the article.

[JT2] L. Schewe, M. Schmidt, and J. Thürauf. "Structural properties of feasible bookings in the European entry-exit gas market system". In: *4OR* 18.2 (2020), pp. 197–218. DOI: 10.1007/s10288-019-00411-3

Based on initial results by Lars Schewe and Martin Schmidt and based on joint discussions, Johannes Thürauf elaborated and extended these results, including new lemmas and proofs. He also wrote main parts of the article.

[JT3] M. Labbé, F. Plein, M. Schmidt, and J. Thürauf. "Deciding feasibility of a booking in the European gas market on a cycle is in P for the case of passive networks". In: *Networks* 78.2 (2021), pp. 128–152. DOI: 10.1002/net.22003

The main ideas for the derivation of the solution approach were developed by Johannes Thürauf and Fränk Plein in discussion with the other authors. Johannes Thürauf contributed theoretical results and proofs that finally led to the main result of this paper. Johannes Thürauf was one of the primary authors of the article.

- [JT4] J. Thürauf. *Deciding the Feasibility of a Booking in the European Gas Market is coNP-hard*. Tech. rep. Submitted. 2020. URL: http://www.optimization-online.org/DB_HTML/2020/05/7803.html

- [JT5] F. Plein, J. Thürauf, M. Labbé, and M. Schmidt. “A bilevel optimization approach to decide the feasibility of bookings in the European gas market”. In: *Mathematical Methods of Operations Research* (2021). Published Online. DOI: 10.1007/s00186-021-00752-y

  The idea to study the feasibility of bookings with linearly modeled active elements using bilevel optimization approaches resulted from the joint discussion of all four authors. Johannes Thürauf and Fränk Plein jointly developed the bilevel approaches in this paper. Fränk Plein contributed the implementation and conducted the computational study. Johannes Thürauf contributed significant parts to the writing of the article.

- [JT6] M. Reuß, L. Welder, J. Thürauf, J. Linßen, T. Grube, L. Schewe, M. Schmidt, D. Stolten, and M. Robinius. “Modeling hydrogen networks for future energy systems: A comparison of linear and nonlinear approaches”. In: *International Journal of Hydrogen Energy* 44.60 (2019), pp. 32136–32150. DOI: 10.1016/j.ijhydene.2019.10.080

  Johannes Thürauf contributed ideas to the implementation of the nonlinear approach and the corresponding computational study. He also contributed to the writing of the article.

- [JT7] L. Schewe, M. Schmidt, and J. Thürauf. “Computing technical capacities in the European entry-exit gas market is NP-hard”. In: *Annals of Operations Research* 295.1 (2020), pp. 337–362. DOI: 10.1007/s10479-020-03725-2

  Johannes Thürauf proposed the research question to consider the computational complexity of technical capacities together with Lars Schewe. He derived and proved the theoretical results and also primarily wrote the article.

- [JT8] L. Schewe, M. Schmidt, and J. Thürauf. “Global optimization for the multilevel European gas market system with nonlinear flow models on trees”. In: *Journal of Global Optimization* (2022). Published Online. DOI: 10.1007/s10898-021-01099-8

  Johannes Thürauf proposed the initial research question to model technical capacities using the underlying network structure. He derived and proved the theoretical results and was responsible for the corresponding implementation. Moreover, he conducted the computational study including the instance generation in joint discussion with the other authors. He also primarily wrote the article.

In addition, the following peer-reviewed article has been written during the author's PhD study. It is not included as part of this dissertation since it slightly differs from the research topic of this dissertation.

[JT9] J. Grübel, T. Kleinert, V. Krebs, G. Orlinskaya, L. Schewe, M. Schmidt, and J. Thürauf. "On electricity market equilibria with storage: Modeling, uniqueness, and a distributed ADMM". in: *Computers & Operations Research* 114 (2020), pp. 104783, 19. DOI: 10.1016/j.cor.2019.104783

Finally, the following article was written and published during the author's PhD studies. Since the main findings of this article result from his master's thesis, the article is not part of the dissertation. However, we would like to note that the author of this dissertation wrote main parts of the article as well as significantly improved the proofs of Section 3 during his PhD studies.

[JT10] M. Robinius, L. Schewe, M. Schmidt, D. Stolten, J. Thürauf, and L. Welder. "Robust optimal discrete arc sizing for tree-shaped potential networks". In: *Computational Optimization and Applications* 73.3 (2019), pp. 791–819. DOI: 10.1007/s10589-019-00085-x

Contents

Part A

Extended Summary

1. Introduction

Many real-life decisions are based on uncertain data for a variety of reasons. One reason may be deviations from predictions or estimations. For example, the future demand for hydrogen is naturally subject to fluctuations and is the base for constructing the corresponding hydrogen infrastructure. Further, it is often too costly or nearly impossible to exactly measure certain parameters, e.g., the roughness of pipelines, which leads to measurement errors in the data. Uncertainties in the data lead to uncertain parameters in optimization models, which in many cases are used to support decision making. From a theoretical as well as a practical point of view, it is of great importance to consider uncertainties in optimization problems since even small perturbations in the data can lead to nonoptimal or even infeasible solutions. For example, studying linear problems of the `NETLIB` collection of real-life examples, it is shown in [16] that perturbations of the input data up to 1 % can make the originally computed solution heavily infeasible.

There are two popular approaches to protect optimization problems against data uncertainties. If the probability distribution of the uncertain parameters is known or can be estimated, then *stochastic optimization* is a popular approach to account for uncertainties in optimization problems. Typically stochastic optimization problems include expectations or so-called chance constraints, which have to be satisfied with a certain probability at least. Since we do not consider this approach in the following, we refer to [24, 104] for details on stochastic optimization. In this cumulative dissertation, we focus on another popular approach to consider uncertainties in optimization problems, namely *robust optimization*. Compared to stochastic optimization, no information regarding the distribution of the uncertain parameters is required in robust optimization. But it is assumed that the uncertainties are within a so-called uncertainty set. This uncertainty set is specified by the decision maker and typically contains infinitely many scenarios. The general goal of robust optimization is to compute a robust solution that is feasible for all realizations of the uncertain parameters inside the given uncertainty set and that is optimal under this condition. The concept of robust optimization was first introduced in [105] and has become more popular since the 1990s; see Chapter 2 for an overview of robust optimization. Based on the initial idea, modified concepts of robust optimization have been developed to provide more flexibility in practice. For example two-stage, respectively adjustable, robust optimization allows for an additional adjustment after the uncertainty reveals; see [115] and Section 2.2. Further, robust optimization has been successfully applied in different fields such as finance, energy, supply chain, or health care as outlined in [52, 115].

Large parts of the literature in robust optimization focus on developing solution methods to compute robust solutions. The choice of the uncertainty set is comparatively less researched. However, it plays an important role since it influences the set of robust feasible solutions, the tractability of solution methods, and the so-called price of robustness [22]. The latter evaluates the difference between the objective value of a robust solution and of a nominal solution. Thus, it can be seen as a notion of the costs for accounting data uncertainties in optimization problems using robust optimization. In many cases, decision makers choose the uncertainty set based on application-driven aspects. However, it can generally be elusive to assume that the exact "size" of the uncertainty set is known prior to the optimization process. Overly large sized uncertainty sets can lead to infeasible robust optimization problems. To prevent robust infeasibility due to the choice of the uncertainty set, it is useful to know the maximal "size" of a given uncertainty set so that there is at least one robust feasible solution. We address this topic of maximal uncertainty sets with robust feasibility guarantee for general mixed-integer linear problems and in the context of gas networks, which we outline in the next section.

1.1. Challenges

For uncertain mixed-integer linear problems (MIPs), we study a specific notion of size: the radius of robust feasibility (RRF). The latter determines a value for the maximal "size" of a given uncertainty set so that a robust solution still exists. One of the main challenges is that the RRF has only been studied for continuous optimization problems in the literature. In addition, the corresponding approaches do not allow "safe" variables or constraints, i.e., variables or constraints that are not affected by any uncertainties. This restriction significantly limits the use of the RRF, especially in applications that usually contain safe variables and constraints. Thus, we also aim at integrating safe variables and constraints into the concept of the RRF and develop corresponding solution approaches.

Moreover, we address the two-stage robust problems of deciding the feasibility of a booking and of computing maximal technical capacities within the European entry-exit gas market system. This market system was introduced as a result of the European gas market liberalization [44–47] with the goal of decoupling transport and trade. Bookings and technical capacities play an important role in achieving this goal and can roughly be described in line with [64] as follows. A booking is a capacity-right contract between gas traders and the transmission system operator (TSO), which allows the traders to inject or withdraw any balanced quantity of gas at specific nodes up to the booked capacities. Technical capacities are nodal capacities determined by the TSO to set upper bounds on the bookings. Consequently, they denote maximal bookable capacities. For bookings as well as technical capacities, the TSO is obliged to guarantee that every balanced load flow within the bookings, respectively technical capacities, can be transported through the network. Except for some technical subtleties, the considered problems correspond to deciding the feasibility, respectively solving, a specific two-stage nonlinear robust optimization problem. This problem aims at computing a maximal uncertainty set of balanced load flows so that each of these load flows can be transported through the network.

We study this robust problem with focus on nonlinear models of gas transport. Hence, one of the main challenges is that the considered two-stage robust problem is nonlinear and nonconvex. In case of active elements in the network, e.g., compressors, it additionally contains challenging adjustable integer variables, which can adjust their value after the uncertainty reveals. Consequently, even deciding its feasibility poses a big challenge. When solving the considered robust optimization problem, our specific uncertainty set depends on continuous decision variables, which is very challenging and leads to a so-called decision-dependent uncertainty set.

1.2. Contributions and Organization

In Part A of this cumulative dissertation, we provide an extended summary regarding our contributions to the radius of robust feasibility (RRF) as well as to the considered robust problems of deciding the feasibility of a booking and of computing maximal technical capacities within the European entry-exit gas market system. A complete description of our results including all proofs is given in the reprints in Part B.

We first introduce the RRF for MIPs and provide sufficient conditions under which the RRF of a MIP and of its continuous relaxation are the same, exploiting common assumptions from the literature. We then extend the RRF to include "safe" variables and constraints, i.e., variables and constraints that are not affected by uncertainty. Afterward, we develop algorithms for computing the RRF for linear and mixed-integer linear problems with safe variables and constraints. We also successfully apply these approaches to compute the RRF for instances of the MIPLIB 2017 library. Based on our results, we propose a framework to integrate choosing the size of a given uncertainty set in the optimization process, which allows to control the price of robustness by adjusting the size of the uncertainty set.

We now turn to the contributions to the considered two-stage robust problems within the European entry-exit gas market system. We analyze structural properties such as (non-)convexity and star-shapedness of the set of feasible bookings and of the set of feasible balanced load flows for different models of gas transport. From the literature [81], it is known that the feasibility of a booking can be decided in polynomial time for tree-shaped networks consisting only of pipes, which can also be derived from our results using a slightly different approach. We further provide a polynomial-time algorithm for deciding the feasibility of a booking in single-cycle networks consisting of pipes only. However, deciding the feasibility of a booking is coNP-hard in general pipe-only networks. We further characterize the feasibility of bookings in so-called active networks that additionally include controllable elements such as compressors and control valves. Based on the approaches for deciding the feasibility of a booking, we provide first results for computing maximal technical capacities in tree-shaped networks consisting only of pipes. Exploiting our results, it is possible to solve a multilevel model of the European entry-exit gas market from the literature [64] for a tree-shaped pipe-only network of real-world size and a nonlinear gas flow model. Finally, we remark that our results can also contribute to further potential-based network problems such as computing a robust diameter selection for tree-shaped hydrogen networks with uncertain demand.

The extended summary is organized as follows. In Chapter 2, we introduce the robust optimization methodology as well as two-stage robust optimization and discuss relevant solution approaches from the literature. Afterward, we summarize our results regarding the radius of robust feasibility in Chapter 3. We discuss basics of stationary gas flows and introduce our models of gas transport using potential-based flows in Chapter 4. On the basis of these models, we formally introduce the considered robust problems of deciding the feasibility of a booking and of computing maximal technical capacities within the European entry-exit gas market system in Chapter 5. We then study the problem of deciding the feasibility of a booking in Chapter 6 and based on these results, we address the problem of computing maximal technical capacities in Chapter 7. In conclusion, we evaluate our contributions and discuss possible future research in Chapter 8.

2. Foundations of Robust Optimization

The main goal of (strict) robust optimization is to compute a solution that is feasible for all realizations of the uncertain parameters in a user-specified uncertainty set and that is optimal under this condition. The initial idea of robust optimization was introduced in [105] and became more popular in the 1990s; see e.g., [11, 12, 42, 43, 79]. The increased interest in robust optimization continues to this day and leads to a large variety of robust optimization approaches for different optimization problems; see e.g., the book [13] together with the survey articles [15, 18, 29, 52, 61, 83, 115] and the references therein. Robust optimization has been further successfully implemented for different applications such as finance, energy, supply chain, health care as outlined in [52, 61].

In the following, we introduce the classical concept of strict robust optimization in Section 2.1. We then discuss the concept of two-stage or adjustable robust optimization in Section 2.2, in which the numerical values of some decision variables can be specified after the realization of the uncertainties. Afterward, we discuss the choice of the uncertainty set with focus on its size in Section 2.3.

We note that further concepts of robust optimization were developed, e.g., light robustness [49] or distributional robustness [39, 112]. However, in this short introduction to robust optimization, we focus on strict and two-stage robust optimization since we consider these concepts in the subsequent chapters.

2.1. Strict Robust Optimization

We briefly review the classical concept of strict robust optimization[1] (strict RO). The content of this section is based on the book [13] and on the (survey) articles [14, 15, 18, 61], which we also recommend together with [52, 83] for further insights in strict RO. In the following, we consider an optimization problem of the form

$$\min_{x \in \mathbb{R}^n} \left\{ f(x) \,:\, g_i(x, \zeta) \leq 0,\; i \in \{1, \ldots, m\} \right\}, \tag{2.1}$$

where $x \in \mathbb{R}^n$ are the variables of the optimization problem, $f \colon \mathbb{R}^n \to \mathbb{R}$ is the objective function, $g_i \colon \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}$ is a function for $i \in \{1, \ldots, m\}$, and $\zeta \in \mathbb{R}^p$ represents data that specify together with f and g_i for $i \in \{1, \ldots, m\}$ a particular instance of the problem. For ease of notation, we assume that our objective function f is independent from ζ, which is without loss of generality (w.l.o.g.); see e.g., [18]. Problem (2.1) does not contain any uncertainties and is also referred to as the

[1] We note that strict robust optimization is also referred to as static robust optimization in the literature.

nominal problem. The corresponding uncertain problem in strict RO is given by the family of optimization problems

$$\left\{ \min_{x \in \mathbb{R}^n} \{ f(x) \,:\, g_i(x,\zeta) \le 0,\ i \in \{1,\dots,m\}\} : \zeta \in \mathcal{U} \right\}, \tag{2.2}$$

where the data vary in a user-specified uncertainty set $\mathcal{U} \subseteq \mathbb{R}^p$. As briefly discussed in Section 2.3, different choices for the uncertainty set, e.g., discrete, polyhedral, or ellipsoidal sets, are considered in the literature. It is often assumed that the uncertainty set is convex and compact, which we also do in this short introduction to robust optimization. We note that for many robust optimization problems, we can w.l.o.g. replace the uncertainty set by its convex hull, e.g., for uncertain convex problems with concave uncertainty; see [11]. However, this is generally not possible for uncertain nonlinear optimization problems.

As described in [13], the main goal of strict RO consists of computing a solution x of "here-and-now" decisions before the uncertainty "reveals itself" such that this solution x is "immunized" against all realizations within the uncertainty set. This leads to the so-called strict robust counterpart of the uncertain problem (2.2), see e.g., [15], that is given by

$$\min_{x \in \mathbb{R}^n} \{ f(x) \,:\, g_i(x,\zeta) \le 0 \ \forall \zeta \in \mathcal{U},\ i \in \{1,\dots,m\}\}. \tag{2.3}$$

We note that a feasible, respectively optimal, solution for the robust counterpart (2.3) is called a robust feasible, respectively robust optimal, solution for the uncertain problem (2.2). Consequently, a robust feasible solution is immunized against all possible realizations within the uncertainty set $\mathcal{U}$. Usually the uncertainty set $\mathcal{U}$ contains infinitely many elements. Thus, the robust counterpart (2.3) turns out to be a semi-infinite problem.

Many approaches for solving robust counterparts have been developed; see e.g., the book [13] and the articles [14, 18, 61, 83] for a comprehensive overview. In this short introduction to strict RO, we briefly highlight two popular approaches for solving robust counterparts, namely a duality based reformulation technique and the so-called adversarial approach. As discussed in [13, 18], we can w.l.o.g. assume in strict RO that the uncertainty is given constraint-wise, i.e., the uncertainty set $\mathcal{U}$ has the form $\mathcal{U} = \mathcal{U}_1 \times \dots \times \mathcal{U}_m$, where, for $i \in \{1,\dots,m\}$, the set $\mathcal{U}_i$ is the projection of the uncertainty set $\mathcal{U}$ on the space of the data of the ith constraint. Thus, we can w.l.o.g. assume that the constraints of the robust counterpart are given by

$$g_i(x,\zeta) \le 0 \quad \forall \zeta \in \mathcal{U}_i,\ i = \{1,\dots,m\}. \tag{2.4}$$

The first approach we discuss uses duality-based arguments in order to obtain an equivalent and finite-dimensional reformulation of the usually semi-infinite robust counterpart (2.3), i.e., the reformulation consists of finitely many variables and constraints. In this dissertation, we call such a finite-dimensional reformulation algorithmically tractable. We only sketch the basic idea of the reformulation technique, which is one of the main approaches in strict RO, and refer to e.g., [13, 14, 18, 115] for more details. The approach consists of three main steps and can usually be applied to robust optimization problems in which the constraint functions g_i and the uncertainty set $\mathcal{U}_i$ satisfy certain convexity and regularity conditions; see e.g., [14] for details on the requirements. Our description of these three steps follows the one in [14, 115].

As first step, we consider the *worst-case* regarding the ith uncertain constraint of (2.4), which can be formulated as

$$\max_{\zeta \in \mathcal{U}_i} g_i(x, \zeta) \leq 0. \tag{2.5}$$

As second step, we can equivalently replace the maximization problem of the left-hand side in (2.5) by its dual problem under certain convexity and regularity conditions on the constraint function g_i and the uncertainty set $\mathcal{U}_i$; see e.g., [14]. This leads to a reformulation of (2.5) in which the maximization problem is now replaced by an equivalent minimization problem. In a third step, we can eliminate this minimization expression since it suffices that at least one feasible point of the dual minimization problem satisfies the reformulated constraint. For an overview of reformulated robust counterparts with respect to (w.r.t.) different uncertainty sets and constraints, we refer to [14] and [13]. We note that the reformulation approach can directly be applied to uncertain mixed-integer linear problems since the duality arguments are applied regarding the uncertainty set for fixed optimization variables x.

As second approach to solve robust optimization problems, we briefly sketch the main idea of the adversarial approach; see [23]. We follow its description given in [115]. The core idea of the adversarial approach consists of replacing the original uncertainty set $\mathcal{U}$ by a finite set of scenarios $S \subseteq \mathcal{U}$. At the beginning, a user-specified set of finitely many scenarios $S \subseteq \mathcal{U}$, e.g., the nominal scenario, is chosen. Then, we solve the robust counterpart w.r.t. the finite scenarios within S, i.e., we replace $\mathcal{U}$ by S in (2.3). Consequently, the modified robust counterpart consists of finitely many variables and constraints. If the corresponding solution is robust feasible, then it is also a robust optimal solution due to $S \subseteq \mathcal{U}$. Otherwise, scenarios in $\mathcal{U} \setminus S$ exist for which the computed solution is infeasible. If this is the case, then one of these scenarios is added to S and the approach iterates again by solving the corresponding robust counterpart w.r.t. S. We note that we can find one of these scenarios that violates the computed solution by maximizing the violation of the constraints w.r.t. the uncertainty set. However, it may be necessary to solve these subproblems to global optimality in order to find a scenario that violates the computed solution, which can be challenging, especially for the case of nonconvex problems. For more details regarding the adversarial approach, we refer to [23]. In practice the adversarial approach often performs well even if it is not guaranteed that it terminates after a finite number of iterations in general. However, for linear constraints and a polyhedral uncertainty set, the adversarial approach terminates after a finite number of iterations; see e.g., [21]. For a comprehensive computational study that compares the adversarial approach and the sketched robust reformulation techniques, we refer to [21].

After introducing the basics of strict robust optimization, we now turn to the concept of two-stage robust optimization in the next section. This concept relaxes the condition of strict robust optimization that every decision has to be made before the uncertainty materializes. Thus, in two-stage robust optimization it is possible to adjust specific decisions to the realization of the uncertainty, which is necessary, respectively beneficial, in some applications. For example, in the later considered gas networks pressure levels are adjusted to uncertain demand.

2.2. Two-Stage Robust Optimization

A two-stage robust optimization problem[2] usually contains so-called "here-and-now" and "wait-and-see" decisions. As in strict RO, the "here-and-now" decisions have to be made before the uncertainty reveals itself. In contrast to this, the "wait-and-see" decisions can be adjusted with knowledge of the realization of the uncertainty. On the one hand, two-stage robust optimization is generally less conservative w.r.t. the optimal objective value than the strict RO approach since it allows for a reaction to the revealed uncertainty at a later stage. On the other hand, this additional flexibility leads to algorithmically challenging optimization problems. For example, even for linear problems with polyhedral uncertainty two-stage robust optimization is NP-hard, see [67], in contrast to the corresponding strict robust optimization problem [12].

In analogy to (2.3) in strict RO, we now introduce the two-stage robust counterpart and discuss some solution approaches for it. The material of this section is based on the book [13, Chapter 14] and the recent survey article [115], which we recommend for further insights. The two-stage robust counterpart is given by

$$\min_{x\in\mathbb{R}^n} \left\{ f(x) \,:\, \exists x \in \mathbb{R}^n \ \forall \zeta \in \mathcal{U} \ \exists y \in \mathbb{R}^k : g_i(x,\zeta,y) \le 0, \ i \in \{1,\dots,m\} \right\}, \tag{2.6}$$

where $x \in \mathbb{R}^n$ are the first-stage, respectively "here-and-now", decisions, which are made before the uncertainty reveals itself. After the realization of the uncertainty $\zeta \in \mathcal{U} \subseteq \mathbb{R}^p$, the second-stage adjustable variables $y \in \mathbb{R}^k$ are chosen such that x and y satisfy $g_i(x,\zeta,y) \le 0$ for all $i \in \{1,\dots,m\}$. We can w.l.o.g. assume that the objective function depends only on the first-stage variables; see [13]. In contrast to strict RO, the uncertainty is generally non-constraint-wise in two-stage robust optimization. As common in adjustable robust optimization, the two-stage robust counterpart can alternatively be defined by using a decision rule $y(\cdot)$, which is a function $y\colon \mathbb{R}^p \to \mathbb{R}^k$ that maps the uncertainties to the space of the adjustable variables. This function is usually unknown prior to the optimization and is specified within the optimization process. Using the notion of decision rules, the two-stage robust counterpart is given by

$$\min_{x\in\mathbb{R}^n,\ y(\cdot)\in Y} \left\{ f(x) \,:\, g_i(x,\zeta,y(\zeta)) \le 0 \ \forall \zeta \in \mathcal{U}, i \in \{1,\dots,m\} \right\}, \tag{2.7}$$

[2]We note that two-stage robust optimization is also referred to as adjustable robust optimization in the literature. Often this is the case for linear problems or if the "wait-and-see", respectively adjustable, decisions are represented by so-called decision rules.

where the set Y consists of all functions that map the uncertainty to the adjustable variables. We now briefly highlight some solution approaches following the descriptions within the recent survey article [115], to which we refer for a detailed overview regarding adjustable robust optimization.

One approach to simplify, respectively approximate, two-stage robust optimization problems consists of restricting the set of possible decision rules Y to specific classes of functions, see e.g., [13, 115]. For example in [10], the decision rules are restricted to affine functions for an uncertain linear problem (LP), i.e., $y(\zeta) = y^0 + Q\zeta$ with $y^0 \in \mathbb{R}^k$ and $Q \in \mathbb{R}^{k\times p}$. Substituting the affine decision rule in (2.7) leads to the so-called affinely adjustable robust counterpart, in which $y^0 \in \mathbb{R}^k$ and $Q \in \mathbb{R}^{k\times p}$ are optimization variables. For the case of fixed recourse, i.e., the coefficients of the adjustable variables are certain, this affinely adjustable robust counterpart can be recast as a computationally tractable optimization problem under certain conditions; see [10]. However, for the case of non-fixed recourse, i.e., products of uncertain coefficients and second-stage variables exist, solving the latter problem is NP-hard; see [10]. An overview of further classes of decision rules studied in the literature is given in Table 3 in [115]. Restricting the decision rules to predefined classes of functions generally leads to solutions that are an upper bound for the original two-stage robust problem (2.7). However, for some classes of adjustable robust optimization problems it is known that specific structures of decision rules are optimal; see [115, Section 4.2].

In many applications some adjustable variables need to be integral, e.g., in some of the later considered robust gas network problems. Different approaches that deal with adjustable integer variables are developed in the literature; see [115, Section 6] for a comprehensive summary. For example, the concept of K-adaptability can be applied to the case of integer adjustable variables. To do so, K second-stage decisions are selected in the first stage and then the best one of them is chosen as response to the observed realization of the uncertainty; see e.g., [19, 28, 70, 106]. A different approach focuses on splitting the uncertainty set into different subsets and allowing specific decisions for each of these sets; see e.g., [20, 93]. This leads to a robust optimal value that is at least as good as the one of the corresponding strict robust optimization problem.

Furthermore, two-stage robust nonlinear models, respectively nonlinear decision rules, are often necessary to accurately model specific applications. This is often the case if the application includes aspects that follow physical laws, e.g., the transport of gas or water in pipeline networks. One approach for the case of fixed recourse applies a nonlinear transformation that moves the nonlinearity from the decision rule to the uncertainty set; see [13, Chapter 14] and [115]. However, computing the convex hull of the transformed uncertainty set can be challenging; see [13, Chapter 14]. Under certain convexity assumptions, the authors in [99] propose a dual approach for two-stage robust nonlinear optimization problems. Two approaches for deciding robust feasibility and infeasibility for two-stage nonlinear robust problems with empty first-stage and additional uniqueness assumption on the second-stage variables are developed in [5] using methods of polynomial optimization. In general, it is often necessary to exploit problem-specific knowledge to obtain solution approaches for two-stage robust nonlinear problems.

Following the idea of the adversarial approach, the so-called scenario approach replaces the uncertainty set of a two-stage robust problem by finitely many realizations of the uncertainty, respectively scenarios. This approach generally leads to a lower bound of the two-stage robust counterpart; see [69]. For the case of adjustable robust linear optimization with a polyhedral uncertainty set, the scenario approach is further extended in [7] by iteratively adding new scenarios to the considered set of finitely many realizations of the uncertainty. Furthermore, adjustable robust nonlinear problems with polytopic uncertainty sets are studied in [108] and a single-level reformulation using finitely many scenarios of the uncertainty set is proposed under specific quasiconvexity assumptions. The finite scenario approach often works well in practice but sometimes the number of necessary scenarios may be very large.

Finally, we note that two-stage robust optimization plays an important role in a wide range of applications such as scheduling, network design, and especially energy problems; see [115, Section 9] for a comprehensive overview and the corresponding literature. We study a specific two-stage nonlinear robust optimization problem in the context of gas networks in Chapters 5–7.

2.3. Choosing the Size of an Uncertainty Set

As briefly summarized in the previous two sections, a large part of research in robust optimization focuses on developing algorithmically tractable robust counterparts and corresponding solution methods. However, the choice of the uncertainty set also plays an important role since it generally affects the set of robust feasible solutions, the tractability of the robust counterpart, and the so-called price of robustness [22]. One of the main goals of choosing the uncertainty set is to avoid too conservative, intractable, or even infeasible robust optimization problems.

As outlined in [13, Chapter 2], specifying an uncertainty set is an important modeling task, which should usually be solved on the basis of the considered application. A variety of different uncertainty sets have been studied in the literature. In many cases the considered uncertainty sets belong to the class of discrete, polyhedral, or ellipsoidal sets; see [85] for a geometric study and [29] for a combinatorial study regarding common uncertainty sets. However, the authors of [13] point out a not necessarily application-driven special case of constructing uncertainty sets, in which the choice of the uncertainty set allows for certain probability guarantees if specific distributional assumptions are satisfied. This is motivated by chance constraints, which are constraints that have to be satisfied with a probability of at least a certain level and can be approximated using robust optimization with a specific choice of the uncertainty set; see e.g., [13, 61]. Since we do not consider this application of robust optimization in the following, we refer to the survey article [61, Section 3] for more details about this approach.

In this dissertation, we focus on choosing the "size" of a given uncertainty set. To do so, we assume that an uncertainty set is given, but its exact size is not specified.

Determining the size of the uncertainty set may then be part of the optimization process. One benefit of this procedure is that the decision maker does not need to determine the exact size of the uncertainty set prior to the optimization procedure, which may be challenging.

One notion for the size of an uncertainty set is based on scaling the uncertainty set. More precisely, the size of a given uncertainty set $\mathcal{U}$ is represented by a nonnegative factor $\alpha \geq 0$ that scales $\mathcal{U}$, i.e., $\alpha\mathcal{U}$ is the uncertainty set in the robust optimization problem. This notion of size is studied from different perspectives in the literature, which we briefly discuss in the following. The authors of [34] investigate how robust solutions change depending on the size of the uncertainty set, to which the authors refer as variable-sized robust optimization. They study how to find a minimal set of robust solutions such that for each size of the uncertainty set, there is at least one robust solution within the computed set of candidate solutions. The authors further study how large an uncertainty set can be increased such that the nominal optimal solution is robust optimal. The authors of [33] develop a method of computing a robust solution that performs well w.r.t. different scaled sizes of a given uncertainty set. Further, the sensitivity of robust solutions w.r.t. changing the size of the uncertainty is studied in [38]. We note that in [33, 34, 38] the focus is on uncertain objective functions, and thus, changing the size of the uncertainty set does not affect the feasibility of the uncertain optimization problem. Moreover, the radius of robust feasibility uses the considered notion of scaling to determine the largest size of the uncertainty set such that a robust feasible solution still exist. To this end, the considered uncertain problem contains uncertain constraints and, thus, the feasibility of the uncertain problem is affected by the size of the uncertainty set. Since we study the radius of robust feasibility in Chapter 3, we refer to this chapter for more details on this approach including the corresponding literature and applications.

Another more general concept of specifying the size of an uncertainty set is given by so-called decision-dependent uncertainty sets, which are also referred to as endogenous uncertainty [82]. A decision-dependent uncertainty set $\mathcal{U}(x)$ depends on decision variables x. Thus, it may change its shape and size considering different solutions. For linear robust optimization problems, two general approaches for decision-dependent polyhedral uncertainty sets are given in [82, 89]. These approaches obtain reformulations that are derived by duality arguments and linearization of bilinear products [89] or implication constraints [82]. We note that both approaches exploit a specific discrete dependency between the optimization variables and the uncertainty set. Decision-dependent uncertainty sets are also studied for different combinatorial optimization problems; see e.g., variable cost uncertainties [92] or the case of combinatorial problems with knapsack uncertainties [91]. In the recent article [117], a decision-dependent uncertainty set is used to introduce a specific notion for the size of an uncertainty set, which is very similar to scaling the uncertainty set. The authors focus on uncertainty sets that are based on how well the parameters are estimated by a so-called estimation metric, i.e., they consider uncertainty sets of the form

$$\mathcal{U}(r; \mathcal{D}) = \{\beta \in \mathcal{W} \subseteq \mathbb{R}^m \colon \rho(\beta; \mathcal{D}) \leq \hat{\rho} + r\}, \tag{2.8}$$

where $\rho(\beta; \mathcal{D})$ is referred to as the estimation metric, $\mathcal{D}$ represents given data, and $\hat{\rho} \in \mathbb{R}$ is a constant. Given this estimation, they maximize the size of the uncertainty set, i.e., they maximize $r \geq 0$, such that the robust problem is still feasible. We note that the concept proposed in [117] is very similar to the radius of robust feasibility; see Chapter 3. In general, decision-dependent uncertainties are of interest in many different applications such as scheduling [110], energy networks [2], or health care [117]. We further study a two-stage nonlinear optimization problem with a decision-dependent uncertainty set depending on continuous first-stage variables in the context of gas networks in Chapter 7.

Finally, we note that decision-dependent uncertainty sets generally allow a greater flexibility to adjust the size of an uncertainty set during the optimization process compared to the notion of scaling the uncertainty set. However, it is often necessary to exploit problem-specific knowledge or assume strong additional assumptions to solve robust optimization problems with decision-dependent uncertainties.

In the next chapter, we study the previously mentioned radius of robust feasibility for general mixed-integer problems.

3. Radius of Robust Feasibility for Mixed-Integer Problems

In this chapter, we summarize and discuss our results of [JT1] regarding a specific notion of size of a given uncertainty set: the radius of robust feasibility (RRF). For a complete description of our results including all proofs, we refer to [JT1], on which this chapter is based. The RRF determines the maximal size of a given uncertainty set so that at least one robust feasible solution exists. To do so, it considers the concept of strict robust optimization. In a nutshell, the RRF is defined as the supremum over all scaled sizes of a given uncertainty set so that a robust feasible point still exists.

We provide a first intuition for the RRF by the following preliminary example, which is an adapted version of Example 2[1] in [JT1]. For fixed $\alpha \geq 0$ and uncertainty set $\mathcal{U} = [-1, 1]^3$, we consider the uncertain constraints

$$\begin{aligned} (-1 + u_1)x_1 + (-2 + u_2)x_2 &\leq 0.5 - u_3 \ \forall u \in \alpha\mathcal{U}, \\ (-1 + u_1)x_1 + (2 + u_2)x_2 &\leq 2.5 - u_3 \ \forall u \in \alpha\mathcal{U}, \\ 0 \leq x_1 &\leq 3, \end{aligned} \tag{3.1}$$

where the first and second constraint are affected by uncertainties and the third one not, i.e., the latter constraint is called "safe". The RRF now equals the supremum of α so that robust feasibility of (3.1) is still guaranteed. As to expect, the set of robust feasible points decreases if the size of the uncertainty set, i.e., $\alpha \geq 0$, increases; see Figure 3.1. The RRF of (3.1) equals 1 and $x_1 = 0, x_2 = 0.5$ is a feasible solution. If we restrict the variables x_1 and x_2 to be integer, i.e., $x_1, x_2 \in \mathbb{Z}$, then the RRF is given by 0.875 and $x_1 = 3, x_2 = 0$ is a feasible solution. We note that the RRF does not change the shape of the uncertainty set $\mathcal{U}$, e.g., a cube remains a cube after scaling; see Figure 3.1.

We now briefly discuss approaches from the literature regarding the RRF, which summarizes and extends our corresponding literature review within [JT1]. In the literature, the RRF has been studied for continuous optimization problems with full-dimensional uncertainty sets, i.e., every constraint and variable is affected by uncertainties. In [36, 57, 58], the case of linear problems (LPs) is studied w.r.t. different convex and compact uncertainty sets. The authors of [56] introduce the RRF in robust convex optimization, and corresponding methods for its computation are provided in [35, 56, 84]. In doing so, the authors of [35] develop first results for the case that each constraint has its own uncertainty set, which may differ from each other. In [60], the RRF for uncertain linear conic programs is studied and computable lower and upper bounds using semidefinite linear programs are provided.

[1] Throughout this chapter, the referenced numbers refer to ones in the published version of [JT1].

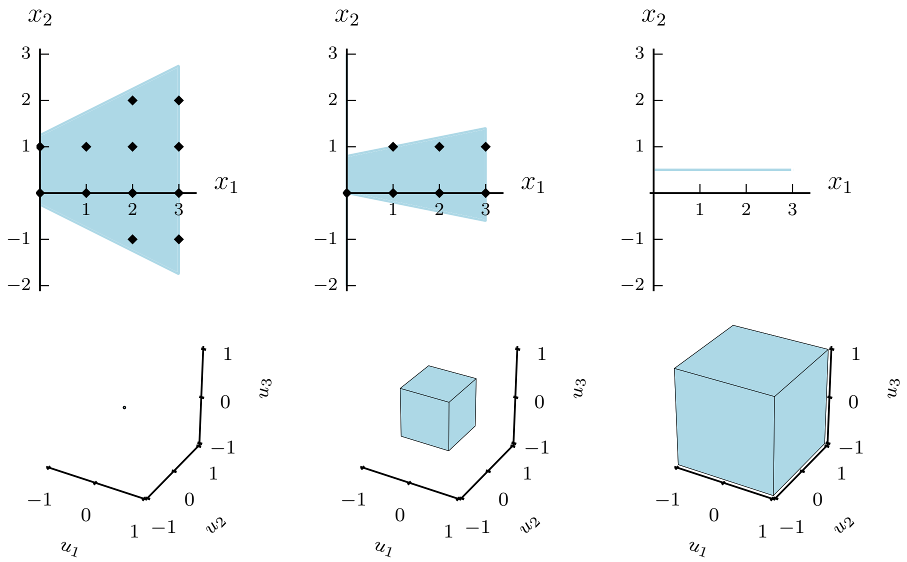

Figure 3.1.: (Top) Set of robust feasible points of (3.1) for the uncertainty sets $0\mathcal{U}$ (left), $0.5\mathcal{U}$ (middle), and $1\mathcal{U}$ (right) with $\mathcal{U} = [-1, 1]^3$. The feasible integer points are marked by diamonds. (Bottom) Illustration of the uncertainty sets $0\mathcal{U}$ (left), $0.5\mathcal{U}$ (middle), and $1\mathcal{U}$ (right).

A more detailed literature review regarding the RRF for different classes of uncertain problems is given in the recent survey article [59], which additionally studies the connection between the RRF and the distance to ill-posedness. In addition, we note that the authors of the recent article [117] introduce a specific notion of size of an uncertainty set, which is very similar to the RRF; see Section 2.3 for details on this notion. One of the differences compared to the RRF is that in [117] the uncertainty set directly depends on the "sizing" variable α, i.e., $\mathcal{U}(\alpha)$ is considered instead of $\alpha\mathcal{U}$. This provides more flexibility to change the size of an uncertainty set, but it may be more difficult to obtain a corresponding robust counterpart. In general, the authors of [117] focus on developing robust counterparts for different estimation procedures and propose a binary search as solution approach. We further note that the RRF arises in specific applications such as facility location design [30, 31], the flexibility index problem [116], or health care [117], in which the considered robust problems can be seen as computing the RRF including safe variables and constraints that are not affected by any uncertainty.

This chapter is outlined as follows. In Section 3.1, we introduce the RRF for mixed-integer linear problems (MIPs) and discuss relations between the RRF of a MIP and its continuous (LP) relaxation in the common setting of the literature, i.e., every variable and constraint is affected by uncertainties. In Section 3.2, we extend the RRF to include "safe" variables and constraints, which are not affected by uncertainty and usually appear in applications. Afterward, we discuss our methods for computing the RRF with safe variables and constraints for LPs and MIPs in Section 3.3 and apply these methods to compute the RRF for instances of the MIPLIB 2017 library in Section 3.4. Based on our results, we propose a framework to integrate sizing the uncertainty set in the optimization process in Section 3.5, which allows to control the price of robustness by adjusting the size of the uncertainty set.

All of the following results of this chapter are taken from [JT1] and we closely follow their corresponding description within [JT1]. We further use the notation of [JT1] throughout this chapter.

3.1. Relations between a MIP and its LP Relaxation

We now formally introduce the radius of robust feasibility (RRF) for MIPs as described in [JT1]. To do so, we consider a feasible MIP with coefficients $\bar{a}^j \in \mathbb{R}^n$ and $\bar{b}^j \in \mathbb{R}$ for the finitely many constraints indexed by $j \in J \subset \mathbb{N}$ and coefficients $c \in \mathbb{R}^n$ of the objective function given by

$$\min_{x \in \mathbb{Z}^k \times \mathbb{R}^{n-k}} \left\{ c^T x \colon (\bar{a}^j)^T x \leq \bar{b}^j, j \in J \right\}. \tag{P}$$

For fixed $\alpha \geq 0$, we denote the robust counterpart for the uncertain MIP (P) with convex and compact uncertainty set $\alpha\mathcal{U} \subseteq \mathbb{R}^{n+1}$ by

$$\min_{x \in \mathbb{Z}^k \times \mathbb{R}^{n-k}} \left\{ c^T x \colon (a^j)^T x \leq b^j \ \forall (a^j, b^j) \in \left\{ (\bar{a}^j, \bar{b}^j) + \alpha u : u \in \mathcal{U} \right\}, j \in J \right\}. \tag{PR$_\alpha$}$$

We note that (PR$_0$) is feasible due to the feasibility of (P). As in [36, 56, 57, 84], we assume that the uncertainty set $\mathcal{U}$ contains zero in its interior.

Assumption 1. *Uncertainty set $\mathcal{U}$ includes zero in its interior, i.e., $0 \in \operatorname{int} \mathcal{U}$.*

Thus, in (PR$_\alpha$) every variable and constraint is affected by uncertainties. We note that one cannot generally guarantee that zero is *in the interior* of the uncertainty set $\mathcal{U}$, e.g., if the projection of $\mathcal{U}$ on a variable consists only of the zero vector.

In analogy to the case of linear problems, see [36, 57], we define the *radius of robust feasibility* (RRF) for the uncertain mixed-integer problem (P) as

$$\rho_{\text{MIP}} := \sup \{\alpha \geq 0 \colon (\text{PR}_\alpha) \text{ is feasible}\}.$$

The definition of the RRF ρ_{MIP} does not guarantee that (PR$_{\rho_{\text{MIP}}}$) is feasible, even for linear problems; see [57, Example 2.2]. However, (PR$_\alpha$) is feasible for all $\alpha \in [0, \rho_{\text{MIP}})$. If (PR$_{\rho_{\text{MIP}}}$) is feasible, we say that the RRF is *attained*, otherwise it is *not attained*. The latter aspect plays an important role in Theorem 3.1.2.

As described in [JT1], we can reformulate the semi-infinite problem (PR$_\alpha$) as the following finite-dimensional problem

$$\min_{x \in \mathbb{Z}^k \times \mathbb{R}^{n-k}} \left\{ c^T x \colon (\bar{a}^j)^T x + \alpha \delta^\star((x, -1)^T \mid \mathcal{U}) \leq \bar{b}^j, j \in J \right\}, \tag{PRC$_\alpha$}$$

where $\delta^\star(y \mid \mathcal{U}) = \sup_{u \in \mathcal{U}} y^T u$ denotes the so-called support function. An overview of explicit formulations for (PRC$_\alpha$) w.r.t. different convex and compact uncertainty sets is given in [14].

Unfortunately, the approaches to compute the RRF of continuous problems, e.g., [35, 36, 56, 84], exploit techniques that cannot generally be transferred to the case of MIPs. Thus, as a first step we study relations between the RRF of (P) and its continuous relaxation (LP relaxation)

$$\min_{x\in\mathbb{R}^n} \left\{ c^T x \colon (\bar{a}^j)^T x \leq \bar{b}^j, j \in J \right\}. \tag{LP}$$

We denote the RRF of (P) by ρ_{MIP} and of its LP relaxation (LP) by ρ_{LP} throughout this chapter. As shown in [JT1] and in line with the initial intuition, the RRF of the LP relaxation (LP) is an upper bound for the RRF of the corresponding MIP (P), i.e., $0 \leq \rho_{\text{MIP}} \leq \rho_{\text{LP}}$. The latter are finite due to Assumption 1; see [57]. We further point out a monotonicity statement w.r.t. the feasibility of (PR_α). It is based on the observation that a robust feasible point is also robust feasible for a subset of the uncertainty set and we algorithmically exploit this property in Section 3.3.

Observation 3.1.1 (Observation 1 in [JT1])**.** *If x is a feasible solution to* (PR_α)*, then x is also feasible for* ($\text{PR}_{\alpha'}$) *for all $\alpha' \in [0, \alpha]$.*

As main result of this section, we reveal a strong connection between the RRF of (P) and of its LP relaxation (LP) under certain conditions.

Theorem 3.1.2 (Theorem 2 i. in [JT1])**.** *Let ρ_{MIP} be the RRF of* (P) *and ρ_{LP} the RRF of its LP relaxation* (LP)*. If the RRF of* (LP) *is not attained, i.e.,* ($\text{PR}_{\rho_{\text{LP}}}$) *is infeasible, then $\rho_{\text{MIP}} = \rho_{\text{LP}}$ holds.*

The benefit of this result is that it provides sufficient conditions so that we can compute the RRF of (P) using known techniques for the RRF of LPs. To do so, we first compute the RRF of the LP relaxation using the approaches of e.g., [36] or Section 3.3. If the resulting RRF is not attained, then it is also the RRF of the corresponding MIP. Otherwise, we yield an upper bound for the RRF of (P), which is necessary for some of the algorithms presented later.

The proof of Theorem 3.1.2 exploits Assumption 1 and constructs for every $\alpha < \rho_{\text{LP}}$ a feasible mixed-integer point of (PR_α) using a sequence of feasible points of the uncertain LP relaxation; see [JT1]. As shown in [JT1], we cannot obtain a result similar to Theorem 3.1.2 if the RRF ρ_{LP} is attained or if we relax Assumption 1, which we do in the next section.

3.2. Extension: Safe Variables and Constraints

In practice, many uncertain optimization problems contain variables and constraints that are not affected by uncertainties. This aspect cannot be taken into account in the common setting of the RRF due to Assumption 1. That motivated us to develop an extended setting of the RRF in Section 3 of [JT1], which allows for so-called safe variables and constraints. We briefly discuss this extended setting of the RRF in the following.

As described in [JT1], for fixed $\alpha \geq 0$ the extended robust counterpart for our uncertain MIP (P) is now given by

$$\min_{x\in\mathbb{Z}^k\times\mathbb{R}^{n-k}} \left\{ c^T x \colon (a^j)^T x \leq b^j \;\; \forall (a^j, b^j) \in \left\{ (\bar{a}^j, \bar{b}^j) + \alpha u : u \in \bar{\mathcal{U}}_j \right\}, j \in J \right\} \tag{EPR_α}$$

where for $j \in J$ the uncertainty set $\bar{\mathcal{U}}_j := \mu^j \, \mathcal{U}_j \subset \mathbb{R}^{n+1}$ is composed of a convex and compact set $\mathcal{U}_j$ that is scaled by the smallest absolute nonzero coefficient μ^j of the jth constraint of (P). The latter prevents that the RRF changes if the nominal constraints are scaled by a scalar; see Lemma 5 in [JT1]. To provide more flexibility regarding the choice of the uncertainty set, we now consider an own uncertainty set for every constraint as in the recent article [35]. However, in contrast to [35], we additionally relax Assumption 1 as follows.

Assumption 2. *Zero is contained in every uncertainty set $\bar{\mathcal{U}}_j$ for $j \in J$.*

If considering the RRF, it is now possible to include "safe" variables and constraints, which are not affected by uncertainties. A decision maker can model a variable x_i for $i \in \{1, \dots, n\}$ as safe in the jth constraint with $j \in J$ by choosing the uncertainty set so that the projection of $\bar{\mathcal{U}}_j$ on the ith axis equals $\{0\}$. Further, the jth constraint with $j \in J$ can be explicitly modeled as safe by choosing the uncertainty set $\bar{\mathcal{U}}_j = \{0\}$. In the following, we use a more general notion of safe constraints introduced in [JT1] that is also called semantically safe and applies for the jth constraint if $\delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) = 0$ holds for all feasible points $x \in \mathbb{R}^n$ of (P). We also denote the index set of the (semantically) safe constraints by S_{MIP}, respectively S_{LP} for continuous linear problems.

In analogy to Section 3.1, we define the RRF in our extended setting as

$$\rho_{\text{MIP}} := \sup \{\alpha \geq 0 \colon (\text{EPR}_\alpha) \text{ is feasible}\}$$

and denote the finite-dimensional robust counterpart of (EPR_α) by

$$\min_{x \in \mathbb{Z}^k \times \mathbb{R}^{n-k}} \left\{ c^T x \colon (\bar{a}^j)^T x + \alpha \delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) \leq \bar{b}^j, j \in J \right\}. \qquad (\text{EPRC}_\alpha)$$

We now point out similarities and differences between the setting of Section 3.1 and our extended setting shown in Section 3 of [JT1]. Unfortunately, the list of desirable similarities is rather short. The only positive results that still hold in our extended setting are that the RRF of the LP relaxation is an upper bound for the RRF of our MIP (P), i.e., $\rho_{\text{MIP}} \leq \rho_{\text{LP}}$, and that the monotonicity statement of Observation 3.1.1 still holds. We now turn to the two major differences regarding the considered settings. First, the main result of the previous section, Theorem 3.1.2, is not satisfied anymore, i.e., we cannot draw the conclusion that if the RRF of the LP relaxation is not attained then it equals the RRF of the corresponding MIP; see Lemma 4 in [JT1]. Second, the RRF is not necessarily finite in our extended setting. We further note that the approaches from the literature for the RRF are based on Assumption 1 and, thus, are not applicable to our extended setting.

To conclude this section, we present a necessary and sufficient optimality condition that holds under additional assumptions. It is based on the rather simple idea that if there is a feasible point such that none of the constraints is tight, then we can increase the size of our uncertainty set. We also algorithmically exploit this result in the next section.

Theorem 3.2.1 (Theorem 4 in [JT1]). *Let the RRF ρ_{MIP} of* (P) *be attained, $S_{MIP} \neq J$ denotes the safe constraints, and for every feasible solution x of* (P) *the inequality $\delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) > 0$ holds for $j \in J \setminus S_{MIP}$. Then, the value α equals ρ_{MIP} if and only if the optimal objective value of*

$$\begin{aligned} \sup_{x,\varepsilon} \quad & \varepsilon \\ s.t. \quad & (\bar{a}^j)^T x + \alpha\delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) + \varepsilon \leq \bar{b}^j, \quad j \in J \setminus S_{MIP}, \\ & (\bar{a}^j)^T x \leq \bar{b}^j, j \in S_{MIP},\ x \in \mathbb{Z}^k \times \mathbb{R}^{n-k},\ \varepsilon \geq 0, \end{aligned} \tag{SPRC$_\alpha$}$$

equals zero.

3.3. Solution Methods that Allow for Safe Variables and Constraints

Since many known approaches from the literature exploit Assumption 1, it is not obvious if and how these methods can be applied to the case of uncertain MIPs with safe variables and constraints. We now briefly discuss our methods of [JT1] for computing the RRF for LPs and MIPs including safe variables and constraints within our extended setting of Section 3.2. We first sketch an approach that computes the RRF for LPs using techniques of fractional programming. Afterward, we present several approaches for the case of MIPs. Throughout this section, we follow the description of the presented approaches of Section 4 in [JT1], to which we refer for more details including all proofs.

3.3.1. Computing the RRF for LPs

Throughout this section and as in [JT1], we consider uncertain linear problems that additionally satisfy the following assumption regarding the uncertainty sets.

Assumption 3. *We assume for our uncertain constraints that, up to scaling, all uncertainty sets are identical, i.e., $\bar{\mathcal{U}}_j = \mu^j\ \lambda^j\ \mathcal{U} \subset \mathbb{R}^{n+1}$ for $j \in J \setminus S_{LP}$ holds, where $S_{LP} \subseteq J$ denotes the index set of our safe constraints, $\mathcal{U}$ is a convex and compact uncertainty set, and λ^j is positive for $j \in J \setminus S_{LP}$.*

This assumption still allows for considering safe variables and constraints. It also covers typical uncertainty sets, e.g., cartesian products; see [JT1].

The main idea of our approach to compute the RRF w.r.t. LPs is based on techniques of fractional programming and can be sketched as follows. Using Assumption 3 and the positive homogeneity of the support function, it is shown in [JT1] that we can compute the RRF of (LP) by solving

$$\sup_{x} \min_{j \in J \setminus S_{\text{LP}}} \frac{\bar{b}^j - (\bar{a}^j)^T x}{\mu^j \lambda^j \delta^\star((x,-1)^T \mid \mathcal{U})} \quad \text{s.t. } (\bar{a}^j)^T x \leq \bar{b}^j,\ j \in S_{\text{LP}}. \tag{3.2}$$

By a priori solving an additional convex optimization problem, we can guarantee that for every feasible point of (LP), each of the corresponding ratios in the objective function of (3.2) consists of a nonnegative and concave numerator as well as a positive and convex denominator; see [JT1]. Thus, Problem (3.2) is a concave generalized fractional program on the set of feasible solution of (LP), see [6, Chapter 7]. In [JT1], it is proven that we can reformulate Problem (3.2) as a concave single ratio fractional program with affine denominator. We then apply a variable transformation, originally stated by Charnes and Cooper [32] and extended in [100] (see also [6]), to obtain a convex reformulation. Solving this convex problem results in the RRF of LPs. We note that for this reformulation to hold, it is necessary that the RRF is positive, which we can ensure by a priori solving an additional linear problem. Overall, the basic structure of our approach can be summarized as follows

(i) Solve a convex optimization problem to detect if there is a feasible solution x of (LP) with $\delta^\star((x,-1)^T \mid \mathcal{U}) = 0$. If this convex problem is feasible, then the RRF is infinite, i.e., $\rho_{\text{LP}} = \infty$.

(ii) Solve a linear problem to check if the RRF is zero. If its optimal objective value is zero, then the RRF equals zero, i.e., $\rho_{\text{LP}} = 0$.

(iii) Solve a convex optimization problem, obtained by applying techniques of fractional programming, to compute the RRF ρ_{LP}.

The complete description of the sketched procedure is given in Algorithm 1 in [JT1] and its correctness is proven by Theorem 5 in [JT1].

Overall, our approach computes the RRF of LPs satisfying Assumption 3 by solving at most two convex and one linear optimization problem.

3.3.2. Computing the RRF of MIPs

We now briefly summarize our different approaches developed in [JT1] for computing the RRF of MIPs in our extended setting of Section 3.2.

By definition the RRF is bounded from below by zero. Throughout this section, we assume that the RRF of (P) is finite and bounded from above by $\bar{u} \in \mathbb{R}$. Using the monotonicity property of Observation 3.1.1 w.r.t. our robust counterpart (EPRC$_\alpha$), we can apply a classic binary search (ClassicBin) on $\alpha \in [0, \bar{u}]$ w.r.t. (EPRC$_\alpha$). This results in an approximation that computes the RRF up to a given tolerance; see Lemma 16 in [JT1]. We now exploit our theoretical results in order to improve the already efficient binary search in practical computations.

Our approaches share a common structure that is illustrated by Algorithm 1 and its explicit components are described in Table 3.1. We improve the classical binary search in ScalingBin and MaxScalingBin by including a scaling argument that tightens the lower bound in each feasible iteration of the binary search; see operation "Lower" in Table 3.1. This scaling maintains the basic properties of the binary search and if a solution x, obtained in an iteration, is also feasible for (EPRC$_{\rho_{\text{MIP}}}$), then this scaling directly sets the lower bound to the optimal RRF ρ_{MIP}; see Lemma 18 in [JT1]. We further include the optimality conditions of Theorem 3.2.1 in MaxScalingBin as an additional termination condition under the assumptions of Theorem 3.2.1. We note that in each iteration we have to solve (SPRC$_\alpha$) to optimality in MaxScalingBin whereas in ScalingBin we only check the feasibility of (EPRC$_\alpha$).

Algorithm 1: Basic Algorithm; taken from [JT1, Algorithm 2][2]

Input: Nominal problem (P), uncertainty sets $\bar{\mathcal{U}}_j$ for $j \in J$, tolerance tol > 0, RRF upper bound $\bar{u}$.

Output: RRF of (P).

Initialization. Init

while Condition **do**

  Update Estimate RRF. Estim

  Solve Subproblem. Subp

  Check Optimality. Optim

  Update Upper Bound. Upper

  Update Lower Bound. Lower

return Results.

Table 3.1.: Overview of algorithms with their specific components in Algorithm 1; taken from [JT1, Table 1] [2].

	ScalingBin	MaxScalingBin	PureScaling
Init	$l \leftarrow 0,\ u \leftarrow \bar{u}$		$l \leftarrow 0$
Condition	$\lvert u - l \rvert > \text{tol}$		$(\text{EPRC}_{(l+\text{tol})})$ feasible
Estim	$\alpha \leftarrow \frac{u+l}{2}$		$\alpha \leftarrow l + \text{tol}$
Subp	$x \leftarrow (\text{EPRC}_\alpha)$	$(\varepsilon, x) \leftarrow (\text{SPRC}_\alpha)$	
Optim		if $\varepsilon = 0$ then return $(\alpha, \mathsf{optimal})$	
Upper	if (EPRC_α) infeasible then $\bar{u} \leftarrow \alpha$	if (SPRC_α) infeasible then $\bar{u} \leftarrow \alpha$	
Lower	$S_{\text{MIP}} \leftarrow \left\{ j \in J \mid \delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) = 0 \right\},\ \ l \leftarrow \min_{j \in J \setminus S_{\text{MIP}}} \frac{\bar{b}^j - (\bar{a}^j)^T x}{\delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j)}$		
Results	l	$(l, \mathsf{non\ optimal})$	

Our final approach PureScaling is similar to MaxScalingBin. As described in [JT1], it combines the scaling argument, operation "Lower" in Table 3.1, and the optimality condition of Theorem 3.2.1 without applying a binary search. To do so, it maximizes the slack in each iteration by solving (SPRC_α) and then updates the current value of the RRF using our scaling argument. The main goal is to detect fast if the current value is close to the RRF and then terminate the procedure without tightening the upper bound of the RRF in many iterations. As we see in the next section this works well in practice.

A specific approach for bounded integer problems that exploits the integrality and big-M constraints to compute the RRF is also developed in [JT1]. In the next section, we analyze the practical performance of our approaches for computing the RRF of MIPs with safe variables and constraints.

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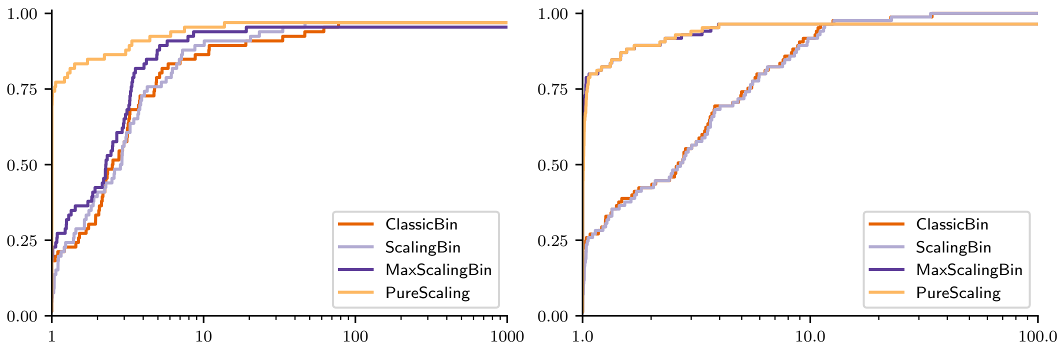

Figure 3.2.: Log-scaled performance profiles of runtimes for 66 instances with positive RRF (left) and for 85 instances with RRF zero (right); taken from [JT1, Figures 1 and 2] [3].

3.4. Computational Study

Section 5 in [JT1] contains a detailed computational study regarding our approaches of Section 3.3.2 for computing the RRF of MIPs using 165 benchmark instances of the MIPLIB 2017 library [55]. In this extended summary, we only focus on two major takeaways of this computational study and refer to [JT1] for the details such as the computational setup and the numerical results. First, we propose a strategy how to compute the RRF using our methods of Section 3.3.2 based on the computational results in [JT1]. Second, we briefly discuss our empirical results regarding the price of robustness [22] if considering the maximal size of the uncertainty set.

As described in [JT1], we suggest the following strategy to compute the RRF of a MIP. First, run PureScaling with a small time or iteration limit. If this does not result in the RRF within the set limit, then we suggest switching to the classic binary search or to ScalingBin since the latter approaches solve more instances overall.

Among others, our strategy is based on the analyzes of log-scaled performance profiles to evaluate runtimes as proposed in [41]. The performance profiles in Figure 3.2 support our presented strategy in line with the detailed numerical results of [JT1] since PureScaling computes the RRF best in short time independent of the value of the RRF. However, classical binary search and ScalingBin, which almost perform equally, solve overall more instances, which lead us to suggest a switch to these methods if PureScaling does not terminate in a set limit. In general, we note that the majority of the instances can be solved quickly (<60 s) and only 14 instances could not be solved within the set time limit of 2 h; see [JT1].

As in [JT1], we finally discuss the price of robustness $p = \frac{w^* - w}{|w|}$, which in our case measures the difference between the optimal objective value w of the nominal problem (P) and the optimal objective value w^* of the robust problem ($\text{EPR}_{\rho_{\text{MIP}}}$) with maximally sized uncertainty set. In the time limit of 2 h, we solved 51 of 66 instances with positive RRF to optimality. Our results in [JT1] show that the price of robustness significantly fluctuates. There are instances with a very low or even zero price of robustness as well as with an extremely large one; see Table 4 in [JT1]. Surprisingly, the median of 384.16 % regarding the price of robustness indicates that

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for many instances the price of robustness is moderate considering the maximal size of the uncertainty set so that robust feasibility is guaranteed. In [JT1], it is empirically shown that increasing the size of the uncertainty set usually leads to an increase of the objective value. However, sometimes there is a chance of increasing the robustness at small or no costs, exemplarily illustrated in [JT1]. Next, we suggest how the RRF can be used to increase the robustness with bounded additional costs.

3.5. Sizing the Uncertainty Set in the Optimization Process

We now propose a framework that allows to simultaneously maximize the size of the uncertainty set and to solve the corresponding robust optimization problem. It also enables the decision maker to control the price of robustness by adjusting the size of the uncertainty set. This idea is briefly mentioned in [JT1] motivated by a bi-objective approach for facility location problems of [31] and we now discuss it in more detail. Our approach is included in the more general concept of inverse robustness as described in the recent article [17]. It is further similar to the joint estimation and robustness optimization framework of [117]. For our uncertain problem (EPR_α) with objective function $c^T x$, our framework consists of the following four steps:

(i) Solve the nominal problem (P) $\rightarrow$ optimal objective value w.

(ii) Define willingness to pay for robustness $\rightarrow$ $B \in \mathbb{R}$.

(iii) Compute the RRF with a safe "budget" constraint, i.e., add the constraint

$$c^T x \leq w + B$$

to (EPR_α) and compute the RRF ρ_{MIP} using our results of Section 3.3.

(iv) Solve ($\text{EPR}_{\rho_{\text{MIP}}}$) to obtain a so-called "most" robust solution.[4]

Our approach computes a "most" robust solution that is protected against all uncertainties within the largest uncertainty set so that the costs do not exceed our set budget for robustness. Thus, the decision maker can control the price of robustness. Moreover, it is only required that the general shape of the uncertainty set, but not its exact size, is determined before the optimization process. To conclude, we note that our approach is also applicable if the decision maker is not willing to pay anything for a robust solution. To do so, the decision maker sets the budget $B = 0$, applies our approach, and may obtain a "most" robust solution for "free".

In the following chapters, we study the two-stage robust problems of deciding the feasibility of a booking as well as of computing technical capacities within the European entry-exit gas market system. The core difficulty of determining technical capacities consists of computing a "maximal" uncertainty set of balanced load flows. However, the maximal uncertainty set is not determined by scaling as it is the case for the RRF. Instead the uncertainty set depends on the decision variables, which leads to a decision-dependent uncertainty set. In the next chapter, we introduce basics of gas transport and our corresponding mathematical models before we formally introduce the considered two-stage robust problems in Chapter 5.

[4] We note that if the RRF is not attained in step (iii), then for an arbitrary small $\varepsilon > 0$ we should consider ($\text{EPR}_{\rho_{\text{MIP}}-\varepsilon}$) in step (iv) in order to avoid infeasibility.

4. Foundations of Stationary Gas Transport Modeled by Potential-Based Flows

In this chapter, we discuss basics of gas transport and introduce different gas flow models, which we then consider throughout this dissertation. We first give a short description of specific components of gas networks in Section 4.1. Afterward, we introduce the considered models of stationary gas transport for pipe-only networks in Section 4.2. We then extend one of these models by linearly modeled compressors and control valves in Section 4.3. The presented models correspond to the ones in [JT2]–[JT5], [JT7], and [JT8]. On the basis of these models, we introduce and study the two-stage robust problems of deciding the feasibility of a booking and of computing technical capacities within the European entry-exit gas market system in Chapters 5–7.

4.1. Gas Network Components

We now briefly describe basic components, namely pipes, compressors, and control valves, that commonly occur in gas networks and that we consider in our models of gas transport in Sections 4.2 and 4.3. The content of this section is based on [50] and the book [77], to which we also refer for a more detailed overview.

Pipes

Gas networks mostly consist of pipelines (pipes for short). The length L and the diameter D are two important parameters of a pipe that influence the gas dynamics. For a fixed quantity of flow, the pressure difference between the endpoints of the pipe increases as the pipeline length is increased or the diameter is decreased. The pressure drop within a pipe is mainly caused by friction, which results from the roughness of the material of the inner pipe wall.

As in [50], we restrict ourselves to the case of cylindrical pipes and one-dimensional flow in the pipes. The gas dynamics within a single pipe can be represented by nonlinear hyperbolic partial differential equations, see [48, 86], which are often called Euler equations. They consist of a continuity, a momentum, and an energy equation. We consider stationary (steady state) models for gas transport throughout this dissertation. We further focus on the isothermal case, i.e., we neglect changes in the gas temperature, and we consider a single type of gas, i.e., we do not take into account effects of mixing different types of gas.

As shown in [50], it is possible to solve the Euler equations in the stationary and isothermal case under the following additional assumptions: the gas temperature and compressibility factor can be approximated by suitable mean values T_m and z_m, the pipes have a constant slope, and the so-called ram pressure term in the momentum equation of the Euler equations is dismissed since its impact is rather small; see [50, 113]. Under these assumptions, we can approximate the gas dynamics in a horizontal pipe, as described in [50], by

$$p_\mathrm{in}^2 - p_\mathrm{out}^2 = \Lambda\,|q|\,q, \tag{4.1}$$

where p_out and p_in describe the pressure levels at the endpoints of the pipe and q represents the flow through the pipe. Further, $\Lambda > 0$ is a pipe specific pressure drop coefficient that is given as follows

$$\Lambda = \left(\frac{4}{\pi}\right)^2 \lambda(q) \frac{R_\mathrm{s} z_\mathrm{m} T_\mathrm{m} L}{D^5}, \tag{4.2}$$

where R_s is the specific gas constant, D denotes the diameter of the pipe, and $\lambda(q)$ represents the friction factor. The latter can be approximated independently from the flow by the formula of Nikuradse [88]. For details about computing the physical parameters in (4.2) as well as the case of non-horizontal pipes, we refer to [50]. The stated relation (4.1) is also known as the *Weymouth equation*; see [111].

Compressor Machines and Control Valves

Compressors machines (compressors for short) are complex elements of the network that allow to increase pressure levels. Thus, compressors play an important role in compensating the pressure loss due to friction when transporting gas over long distances. They also contribute a large part to the operating costs of a gas network. A large variety of modeling compressors in the literature exists, which ranges from linear to sophisticated nonlinear ones. Since we focus on pipe-only networks and networks with linearly modeled compressors and control valves in this dissertation, we exemplarily refer to [50, 54, 97] for specific nonlinear models of compressors.

In our models, we also consider remotely controlled valves (control valves for short). In general, control valves are elements that allow network operators to regulate gas flows and pressure levels. If a control valve is active, it can decrease pressure levels by a certain amount within its a priori defined operation range. For more details on compressors and control valves, we refer to [50, 101]. The linear model for compressors and control valves that we consider in this dissertation is presented in Section 4.3.

Compressors and control valves are actively controlled by a network operator. Thus, they belong to the so-called active elements of the network. We note that usually compressors and control valves can only modify pressure levels if the flow passes through the pipe in a predetermined direction. To model this aspect, binary variables are generally necessary, which is not the case in pipe-only networks.

4.2. Models for Pipes

We now introduce three different models for stationary gas transport in networks consisting only of pipes. Pipe-only networks are also called *passive networks*. The first model is the most general one and is based on general potential-based flows, which form an extension of classical network flows. We then consider a specification of this model based on the Weymouth pressure drop equation (4.1). Finally, we introduce a rather simplified model for gas transport that is based on capacitated linear flows and neglects pressure levels, respectively potential levels. We note that these models correspond to the ones in [JT2]–[JT4], [JT7], [JT8], as well as [JT10] and we follow their corresponding model descriptions in this section.

All of our models share the following basics. The passive gas network, consisting only of pipes, is represented by a directed and weakly connected graph $G = (V, A)$ with node set V and arc set A, i.e., the undirected graph underlying G is connected. The arcs represent pipes and the nodes are partitioned into entries V_+, exits V_-, and inner nodes V_0. We note that for the case of pipe-only networks we also refer to graph $G = (V, A)$ as a passive network. The consideration of directed graphs is a modeling choice that enables us to interpret the direction of the flow. For an arc $a = (u, v) \in A$, the flow q_a is positive if it flows from u to v, whereas it is negative in case it flows against the orientation of the arc from v to u. Further, flow can be injected at entry nodes $u \in V_+$ and it can be withdrawn at exits nodes $u \in V_-$. In our models, we represent the demand and supply in the network at a single point in time by a load flow.

Definition 4.2.1. A load flow is a vector $\ell = (\ell_u)_{u \in V} \in \mathbb{R}^V_{\geq 0}$ with $\ell_u = 0$ for $u \in V_0$. The set of load flows is denoted by L.

Consequently, a load flow $\ell \in \mathbb{R}^V_{\geq 0}$ specifies the amount of gas that is injected, i.e., ℓ_u for $u \in V_+$, and that is withdrawn from the network, i.e., ℓ_u for $u \in V_-$, at a single point in time. Since we consider stationary gas flows, a load flow has to be balanced.

Definition 4.2.2. A balanced load flow is a vector $\ell \in L$ that additionally satisfies $\sum_{u \in V_+} \ell_u = \sum_{u \in V_-} \ell_u$.

Finally, the only constraint that all of our models share is mass conservation at every node of the network modeled by Kirchhoff's first law, i.e.,

$$\sum_{a \in \delta^{\text{out}}(v)} q_a - \sum_{a \in \delta^{\text{in}}(v)} q_a = \begin{cases} \ell_v, & v \in V_+, \\ -\ell_v, & v \in V_-, \\ 0, & v \in V_0, \end{cases} \tag{4.3}$$

where we used the standard δ-notation for the sets of in- and outgoing arcs, i.e., $\delta^{\text{in}}(v) = \{a \in A \colon a = (u, v)\}$ and $\delta^{\text{out}}(v) = \{a \in A \colon a = (v, u)\}$. We now explicitly present our models that describe for a given balanced load flow $\ell \in L$ the corresponding full problem of gas transport in passive networks.

Our first model corresponds to a general potential-based flow model for the case of passive networks. Potential-based flows form an extension of classical network flows. These flows additionally contain node potentials that are linked to the classical flow variables. On the one side, the coupling of potentials and flows often provides additional structure, e.g., uniqueness of the flows as in Theorem 4.2.1, that can be exploited for solution approaches. On the other side, this coupling is usually nonlinear and, thus, results in challenging nonlinear optimization problems.

For a formal introduction to general potential networks and potential-based flows, we refer to [65]. Potential-based flows have been studied theoretically and practically, especially in the context of energy networks, in which the potentials and flows follow specific physical laws. One of the starting points of this research seems to be [25]. As described in [65], the corresponding research mainly focuses on uniqueness of solutions and the development of algorithms. Examples for results regarding the uniqueness of potential-based flows are given in [37, 87, 95]. For exemplary algorithmic results, we refer to [65, 68] and more generally to [96]. Moreover, potential-based flows have been used in many specific applications such as modeling gas transport; see e.g., [3, 4, 65, 77, 94].

Our potential-based flow model (PBF) consists of flows $q = (q_a)_{a\in A}$ and potentials $\pi = (\pi_u)_{u\in V}$. For every node $u \in V$, lower and upper potential bounds $0 < \pi_u^- \le \pi_u^+$ are given. Furthermore, for every pipe $a \in A$, a *potential function* ψ_a is given for which we assume the following as in [65, 81].

Definition 4.2.3. For a pipe $a = (u, v) \in A$, the potential function ψ_a is a function $\psi_a \colon \mathbb{R} \to \mathbb{R}$ that satisfies the following properties

(i) ψ_a is continuous,

(ii) ψ_a is strictly increasing, and

(iii) ψ_a is odd, i.e., $\psi_a(-q_a) = -\psi_a(q_a)$.

The first two assumptions regarding ψ_a are natural in the context of energy networks. The third assumption makes the situation symmetric w.r.t. the arc flow.

Our first and most general model (PBF) is formally given by

$$\pi_u - \pi_v = \psi_a(q_a), \qquad a = (u, v) \in A, \tag{PBF a}$$

$$\pi_u^- \le \pi_u \le \pi_u^+, \qquad u \in V, \tag{PBF b}$$

$$(4.3). \tag{PBF c}$$

For arc $(u, v) \in A$, the potential function ψ_a links the arc flow q_a to the incident node potentials π_u and π_v by Constraints (PBF a). Usually this coupling of flows and potentials is nonlinear. Due to technical restrictions of the pipes, the potentials have to be in specific ranges, which is ensured by Constraints (PBF b). We note that for a given balanced load flow, a feasible point $(q, \pi; \ell)$ of (PBF) is also referred to as a feasible potential-based flow in a passive network.

One of the main benefits of using general potential-based flows consists of its flexibility w.r.t. its application. In [65], explicit potential functions for stationary gas ψ^{G}, water ψ^{W}, and lossless DC power networks ψ^{DC} are discussed, which result from approximating physical laws. For an arc $a \in A$, they are given by

$$\psi_a^{\mathrm{G}}(q_a) = \Lambda_a q_a \left|q_a\right|, \quad \psi_a^{\mathrm{W}}(q_a) = \Lambda_a \operatorname{sgn}(q_a) \left|q_a\right|^{1.852}, \quad \psi_a^{\mathrm{DC}}(q_a) = \Lambda_a q_a,$$

where $\Lambda_a > 0$ is an arc specific constant that differs for each application.

Our second model is called Weymouth-based flow model (WBF) and is directly derived from (PBF) by using for all $a \in A$ the previously mentioned potential function ψ_a^{G} for the case of gas networks. It represents stationary gas transport for horizontal pipes based on the Weymouth equation (4.1) and is given by

$$\pi_u - \pi_v = \Lambda_a q_a \left| q_a \right|, \qquad a = (u, v) \in A, \tag{WBF a}$$

$$\pi_u^- \leq \pi_u \leq \pi_u^+, \qquad u \in V, \tag{WBF b}$$

$$(4.3), \tag{WBF c}$$

where $\Lambda_a > 0$ is an arc-specific constant for any $a \in A$; see (4.2) for an exemplary choice. In gas networks with horizontal pipes, node potentials correspond to the squared pressure levels at the nodes, i.e., $\pi_u = p_u^2$ for $u \in V$. Keeping this variable transformation in mind, Constraints (WBF a) equals the Weymouth pressure loss equation (4.1), which approximates stationary and isothermal gas dynamics within a pipe; see Section 4.1. Model (WBF) is our main model for gas transport in this extended summary as in [JT2]–[JT4], [JT7], and [JT8]. We note that in some of these article we use an equivalent representation of (WBF) in which the potentials are replaced by the squared pressure levels, i.e., $\pi_u = p_u^2$ for $u \in V$. We further note that our models (PBF) and (WBF) are also capable of handling non-horizontal pipes with constant slopes as explained in [65, Observation 2.2].

Our third and last model (CLF) neglects pressure levels and is based solely on capacitated linear flows. We mainly use this simplified model as auxiliary tool or as a comparison with our potential-based flow models. Further, this type of modeling is also used in some related works w.r.t. the problems considered in Chapters 6 and 7. Our capacitated linear flow model (CLF) is given by

$$q_a^- \leq q_a \leq q_a^+, \qquad a \in A, \tag{CLF a}$$

$$(4.3), \tag{CLF b}$$

where $q_a^- \leq q_a^+$ are given lower and upper arc flow bounds for every arc $a \in A$. As in articles [JT3]–[JT5], [JT7], and [JT8], we neglect these flow bounds in (PBF) and (WBF) since arc flows are implicitly restricted by the potential bounds $\pi^- \leq \pi^+$ due to (PBF a) and (WBF a).

Concluding this section, we state a uniqueness result for potential-based flows in passive networks of the literature, which we also exploit in our approaches later on. If we dismiss potential bounds, then for a given balanced load flow $\ell \in L$ the flows q are uniquely determined by Constraints (4.3) and (PBF a). Further, the corresponding potentials are unique up to a constant shift. This result dates back to the early works [37, 87] and is also obtained in [95] including a proof for the existence of such a solution; see e.g., [3] for a more detailed discussion. We follow the presentation of these results within Chapter [74] of the book [77].

Theorem 4.2.1 (Theorem 7.1 in [74])**.** *Let $G = (V, A)$ be a weakly connected and passive network and let $\ell \in L$ be a balanced load flow, i.e., $\sum_{u \in V_+} \ell_u = \sum_{u \in V_-} \ell_u$.*

Then, there exist potentials $\pi' \in \mathbb{R}^V$ and unique flows $q' \in \mathbb{R}^A$ so that the set of feasible points satisfying Constraints (4.3) and (PBF a) is nonempty and it is given by

$$\{(q', \pi) : \pi = \pi' + \eta \mathbb{1}, \eta \in \mathbb{R}\},$$

where $\mathbb{1} = (1, \dots, 1)^T \in \mathbb{R}^V$ is a vector of ones.

From this result, it directly follows that fixing the potential level of a single node makes a solution of (4.3) and (PBF a) unique. This uniqueness for potential-based flows in passive networks is one of the main differences between the capacitated linear flow model (CLF) and the potential-based models (PBF) and (WBF). Further, in potential-based models no cyclic flow is possible in passive networks, see e.g., [68], in contrast to the capacitated linear flow model.

4.3. Extension: Linearly Modeled Compressors and Control Valves

We now extend our model (WBF) for stationary gas transport in pipe-only networks by including linearly modeled compressors and remote-controlled control valves as described in [JT5]. To do so, we closely follow the description given in [JT5] throughout this section.

As in the case of passive networks, our gas network is represented by a directed and weakly connected graph $G = (V, A)$ with node set V and arc set A. The nodes V are partitioned into entries V_+, exits V_-, and inner nodes V_0. Since we now include compressors and control valves, the set of arcs A is partitioned into pipes A_{pipe}, compressors A_{cm}, and control valves A_{cv}. For ease of notation, we introduce the set $A_{\text{act}} = A_{\text{cm}} \cup A_{\text{cv}}$ that contains all active elements of the network. We note that if the network contains active elements, we also refer to $G = (V, A)$ as an active network. In addition to the flows $q = (q_a)_{a \in A} \in \mathbb{R}^A$ and potentials $\pi = (\pi_u)_{u \in V} \in \mathbb{R}^V$, our model now also includes controls $\Delta = (\Delta_a)_{a \in A_{\text{act}}} \in \mathbb{R}^{A_{\text{act}}}$.

Similar to [3], we consider linearly modeled active elements. A compressor or control valve $a = (u, v) \in A_{\text{act}}$ can linearly modify the potential difference $\pi_u - \pi_v$ by $\Delta_a \in [0, \Delta_a^+]$ if a minimal quantity of flow $m_a \geq 0$ passes through the arc in a predetermined direction, i.e., if $q_a > m_a$ is satisfied. For a given balanced load flow $\ell \in L$, our Weymouth-based flow model for gas transport with linearly modeled active elements, precisely compressors and control valves, is called (WBFA) and it is given by

$$\pi_u - \pi_v = \Lambda_a q_a |q_a|, \quad a = (u, v) \in A_{\text{pipe}}, \tag{WBFA a}$$

$$\pi_u - \pi_v = \begin{cases} -\Delta_a, & a = (u, v) \in A_{\text{cm}}, \\ \Delta_a, & a = (u, v) \in A_{\text{cv}}, \end{cases} \tag{WBFA b}$$

$$0 \leq \Delta_a \leq \Delta_a^+ \chi_a(q), \quad a \in A_{\text{act}}, \tag{WBFA c}$$

$$\pi_u^- \leq \pi_u \leq \pi_u^+, \quad u \in V, \tag{WBFA d}$$

$$(4.3), \tag{WBFA e}$$

where $\chi_a(q)$ is an indicator function of the form

$$\chi_a(q) := \begin{cases} 1, & \text{if } q_a > m_a, \\ 0, & \text{otherwise.} \end{cases}$$

Further, $0 \leq \Delta_a^+$ is an upper bound on the operation range of an active element for all $a \in A_{\text{act}}$. As in the previous section $\Lambda_a > 0$ is a pipe-specific constant for all $a \in A_{\text{pipe}}$ and $0 < \pi_u^- \leq \pi_u^+$ are potential bounds for all $u \in V$. For pipes $a \in A_{\text{pipe}}$, Constraints (WBFA a) couple the potentials of the incident nodes and the corresponding arc flow based on the Weymouth equation (4.1). For the case of active elements $a \in A_{\text{act}}$, the incident node potentials are determined by the corresponding control Δ_a in Constraints (WBFA b). The controls Δ as well as the potentials π are bounded by Constraints (WBFA c) and (WBFA d) due to technical restrictions. As in Section 4.2, the potentials represent the squared pressure levels of the nodes in case of horizontal pipes, i.e., $\pi_u = p_u^2$ for $u \in V$. We note that explicitly modeling the indicator function χ_a generally leads to additional binary variables; see Section 6.5.

The problem of deciding the feasibility of a balanced load flow w.r.t. a given model for gas transport, i.e., deciding the feasibility of the considered model of gas transport, is often referred to as validation of a nomination in the literature. Additionally, determining the cheapest way of transporting a balanced load flow has been studied in literature. For a comprehensive literature review on this topic, we refer to the introductions of [JT2] and [JT3]. We generally note that switching from passive to active networks makes the problem of finding a feasible gas transport for a given balanced load flow even more challenging since it introduces binary variables for switching the active elements on or off. Further, for a given balanced load flow, the flows q determined by (WBFA) are not necessarily unique in contrast to our models (PBF) and (WBF) in passive networks.

In the next chapter, we introduce the two-stage robust problems of deciding the feasibility of a booking and of computing maximal technical capacities within the European entry-exit gas market system, in which the balanced load flow is uncertain. We then study these robust problems w.r.t. the presented models for gas transport in Chapters 6 and 7.

5. The European Entry-Exit Gas Market System: A Two-Stage Robust Challenge

As described in [64], one of the first foundations for the European gas market liberalization was laid by the first European directive [46] with the goal to provide non-discriminatory network access and a market opening. This process was then refined by the second European directive [44] and afterward by the subsequent directive [45] and regulation [47]. As result of the European gas market liberalization, the so-called entry-exit system has been implemented as gas market system in Europe with the goal to decouple transport and trading of gas; see e.g., [63, 64]. For this purpose, the market organization is split into several levels, which are formalized within a multilevel model in [64]. So-called bookings and technical capacities represent core elements of the entry-exit system and can roughly be described in line with [64] as follows. The transmission system operator (TSO) is in charge of the gas transport within the network and interacts with the gas traders via specific capacity-right contracts called bookings. A booking is a mid- to long-term contract that permits the trader to inject or withdraw gas at specific nodes of the network up to the booked capacity. By signing a booking contract, the TSO is obliged to guarantee that each balanced load flow within the booked capacities—generally infinitely many balanced load flows—can be shipped through the network. Moreover, the TSO allocates so-called technical capacities in a preliminary stage in order to specify the capacity which can be booked at each node of the network. Technical capacities bound from above bookings and, thus, describe maximal bookable capacities.

From a mathematical perspective, deciding the feasibility of a booking leads to deciding the feasibility of a specific two-stage robust optimization problem whereas solving the latter subject to additional linear constraints corresponds to computing maximal technical capacities. The latter represents one of the core difficulties of the considered entry-exit gas market system, which we mathematically study in Chapters 6 and 7.

This chapter is outlined as follows. In Section 5.1, we formally introduce the considered two-stage robust problems arising from the European entry-exit gas market system including necessary notations and definitions. Moreover, we sketch the basic structure of the European entry-exit gas market on the basis of the multilevel model of [64]. Afterward, we briefly discuss solution approaches from the literature for the considered two-stage robust problems in Section 5.2.

5.1. The Challenge: Gas Flow with Load Flow Uncertainties

Our subsequent definitions and formal descriptions of deciding the feasibility of a booking and of computing maximal technical capacities closely follows the one in [JT3], [JT5], and [JT7] with minor notational adaptations. As discussed in Chapter 4, we model a gas network by a weakly connected and directed graph $G = (V, A)$, also referred to as network, with nodes V and arcs A. The nodes are partitioned into entry nodes V_+, exit nodes V_-, and the remaining inner nodes V_0. Further, the set of arcs is partitioned into pipes A_{pipe} and active elements A_{act}. We represent the supply and demand at a single point of time by a balanced load flow, see Definition 4.2.2, which is also referred to as a nomination within the entry-exit system.

Definition 5.1.1. A nomination is a balanced load flow $\ell \in L$, i.e., $\ell \in \mathbb{R}^V_{\geq 0}$ with $\ell_u = 0$ for $u \in V_0$ satisfies $\sum_{u \in V_+} \ell_u = \sum_{u \in V_-} \ell_u$. The set of all nominations is formally given by $N := \{\ell \in L : \sum_{u \in V_+} \ell_u = \sum_{u \in V_-} \ell_u\}$.

We note that the terms nomination and balanced load flow are interchangeable and we use them equally in the following. A booking represents a mid- to long-term capacity-right contract between the TSO and gas traders, which permits traders to inject or withdraw any balanced quantity of gas within the booked capacity at specific nodes of the network. The formal description of a booking is as follows.

Definition 5.1.2. A *booking* is a vector $b = (b_u)_{u \in V} \in \mathbb{R}^V_{\geq 0}$, with $b_u = 0$ for all $u \in V_0$. A nomination ℓ is called *booking-compliant* w.r.t. the booking b if $\ell \leq b$ holds, where "$\leq$" is meant component-wise. The set of booking-compliant (or b-compliant) nominations is given by $N(b) := \{\ell \in N : \ell \leq b\}$.

As in [JT2] and [JT7], we now introduce the notion of *feasible nominations* and *feasible bookings*, where "feasible" is meant w.r.t. technical, physical, and legal constraints of gas transport. For ease of notation, we generally represent the considered model of gas transport w.r.t. a given nomination $\ell \in N$ by the constraints

$$c_{\mathcal{E}}(x; \ell) = 0, \quad c_{\mathcal{I}}(x; \ell) \geq 0.$$

These constraints represent one of our usually nonlinear and nonconvex models for stationary gas transport of Chapter 4, which can be reformulated into this form.[1]

Definition 5.1.3. A nomination $\ell \in N$ is *feasible* if a vector $x \in \mathbb{R}^n$ exists so that

$$c_{\mathcal{E}}(x; \ell) = 0, \quad c_{\mathcal{I}}(x; \ell) \geq 0, \tag{5.1}$$

holds. The set of feasible nominations is denoted by F_N.

We now formalize the robust problem of deciding the feasibility of a booking.

Definition 5.1.4. We say that a booking b is *feasible* if all booking-compliant nominations $\ell \in N(b)$ are feasible, i.e., a booking b is feasible if

$$\forall \ell \in N(b)\ \exists x \in \mathbb{R}^n \text{ satisfying } c_{\mathcal{E}}(x; \ell) = 0,\ c_{\mathcal{I}}(x; \ell) \geq 0. \tag{5.2}$$

The set of feasible bookings is denoted by F_B.

[1] We note that we explicitly allow the use of functions such as the indicator function in $c_{\mathcal{E}}(x; \ell) = 0$ and in $c_{\mathcal{I}}(x; \ell) \geq 0$ to represent our gas models of Chapter 4 in this form.

Consequently, for deciding the feasibility of a booking it is generally necessary to check infinitely many booking-compliant nominations for feasibility. From a robust optimization perspective, deciding the feasibility of a booking (5.2) can be seen as a specific two-stage robust feasibility problem. In this robust problem, no first-stage, respectively "here-and-now", decisions occur. The uncertainty set consists of all booking-compliant nominations $N(b)$. For each of these nominations, we have to guarantee that feasible adjustable, respectively "wait-and-see", decisions $x \in \mathbb{R}^n$ for the considered gas transport model exist. However, this is a challenging task since we focus on nonlinear and nonconvex models for gas transport; see (PBF) and (WBF). In case of active elements in the gas network, we additionally have to decide on adjustable integer variables. In Chapter 6, we summarize and discuss our results for deciding the feasibility of a booking.

We now turn to the robust problem of computing maximal technical capacities within the European entry-exit gas market system.

Definition 5.1.5. *Technical capacities* are a vector $q^{\mathrm{TC}} = (q_u^{\mathrm{TC}})_{u \in V} \in \mathbb{R}^V_{\geq 0}$ with $q_u^{\mathrm{TC}} = 0$ for $u \in V_0$. The set of technical capacities is denoted by C.

Technical capacities q^{TC} can also be seen as a booking. However, bookings and technical capacities are determined in the European entry-exit gas market system at different points in time. Thus, we denote them differently. Furthermore, technical capacities represent upper bounds of the bookings.

Definition 5.1.6. We say that technical capacities q^{TC} are *feasible* if all bookings $b \in \mathbb{R}^V_{\geq 0}$ with $b \leq q^{\mathrm{TC}}$ are feasible. The set of feasible technical capacities is denoted by F_{C}.

Consequently, technical capacities $q^{\mathrm{TC}} \in C$ are feasible if and only if all technical capacities-compliant nominations $\ell \in N(q^{\mathrm{TC}})$ are feasible.

In the European entry-exit gas market system, the TSO allocates technical capacities in order to determine the nodal capacities that can be booked by the gas traders at specific nodes of the networks. Consequently, the TSO is interested in computing maximal technical capacities to provide more flexibility for the gas traders. As described in [JT7], the problem of computing maximal technical capacities w.r.t. a fixed weight vector $d \in \mathbb{R}^V$ and a model of gas transport $c_{\mathcal{E}}(x;\ell) = 0$ and $c_{\mathcal{I}}(x;\ell) \geq 0$ is formally given by

$$\max_{q^{\mathrm{TC}} \in C} \quad d^T q^{\mathrm{TC}} \tag{5.3a}$$

$$\text{s.t.} \quad \sum_{u \in V_-} q_u^{\mathrm{TC}} \geq q_v^{\mathrm{TC}}, \quad v \in V_+, \tag{5.3b}$$

$$\sum_{u \in V_+} q_u^{\mathrm{TC}} \geq q_v^{\mathrm{TC}}, \quad v \in V_-, \tag{5.3c}$$

$$\text{s.t.} \quad \forall \ell \in N(q^{\mathrm{TC}}) \ \exists x \in \mathbb{R}^n \text{ satisfying } c_{\mathcal{E}}(x;\ell) = 0,\ c_{\mathcal{I}}(x;\ell) \geq 0. \tag{5.3d}$$

Problem (5.3) can be seen as a two-stage robust optimization problem with decision-dependent uncertainty set $N(q^{\mathrm{TC}})$. The robust optimization task is to compute maximal technical capacities q^{TC} so that every balanced load flow $\ell \in N(q^{\mathrm{TC}})$ can be transported through the network, i.e., for all $\ell \in N(q^{\mathrm{TC}})$ there is a $x \in \mathbb{R}^n$ satisfying $c_{\mathcal{E}}(x;\ell) = 0$ and $c_{\mathcal{I}}(x;\ell) \geq 0$. Consequently, technical capacities q^{TC} represent continuous first-stage variable, also called "here-and-now" decisions, that have to be decided before the load flow uncertainties $\ell \in N(q^{\mathrm{TC}})$ are revealed. Additionally, the technical capacities have to satisfy Constraints (5.3b) and (5.3c). As explained in [JT7], these constraints prevent the computation of "unusable" technical capacities, i.e., node capacities that cannot be nominated in any technical-capacities-compliant nomination. Further, the decisions x w.r.t. the gas transport represent second-stage variables, also called "wait-and-see", decisions, which can be determined after the value of the uncertain load flow $\ell \in N(q^{\mathrm{TC}})$ is known. Since we focus on accurate nonlinear models for gas transport, these adjustable variables have to satisfy challenging nonlinear and nonconvex constraints.

Considering the uncertainty set $N(q^{\mathrm{TC}})$, Problem (5.3) computes a "maximal" size of the load flow uncertainty set $N(q^{\mathrm{TC}})$ so that each of these balanced load flows, respectively nominations, can be transported through the network. Here, "maximal" size is meant w.r.t. the objective function of (5.3), which solely depends on the chosen technical capacities. Since every nomination within $N(q^{\mathrm{TC}})$ has to be feasible, the technical capacities q^{TC} have to be chosen so that the uncertainty set $N(q^{\mathrm{TC}})$ lies within the generally nonconvex set of feasible nominations F_N. We exemplarily illustrate this in Figure 5.2. One of the main differences compared to maximizing the size of an uncertainty set by the radius of robust feasibility (RRF), see Chapter 3, is that the RRF scales a given uncertainty set by a positive factor to increase the size of the uncertainty set. This preserves the original shape of the uncertainty set, e.g., a cube stays a cube after scaling; see Figure 3.1. However, computing maximal technical capacities provides more flexibility for sizing the uncertainty set; see Figures 5.1 and 5.2. More precisely, the obtained uncertainty set $N(q^{\mathrm{TC}})$ is always polyhedral since it results from the intersection of a hyperplane and an interval uncertainty set. The technical capacities allow to independently change the size of each of these intervals, which is not possible using the RRF with a single radius as defined in Chapter 3. However, the flexibility for sizing the uncertainty set within the computation of technical capacities can be imitated by introducing different radii for scaling the uncertainty set within the RRF for two-stage robust optimization problems, which is a not yet studied research field.

Computing maximal technical capacities is equivalent to computing a maximal booking satisfying the additional constraints (5.3b) and (5.3c). Consequently, our approaches for deciding the feasibility of a booking can also be used to decide robust feasibility of (5.3) w.r.t. a given point, which is a first and necessary step for solving the latter. Based on the findings for bookings of Chapter 6, we discuss our results for computing maximal technical capacities in Chapter 7.

We note that the described robust problems regarding bookings and technical capacities only address certain parts of the European entry-exit gas market system. For a more complete overview on this market structure, we refer to [63, 64, 98].

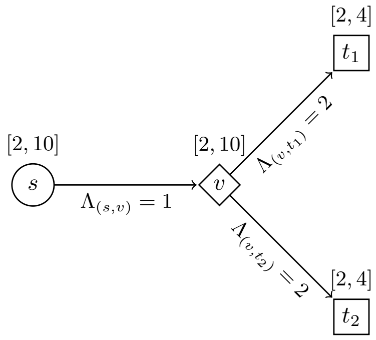

Figure 5.1.: An exemplary instance for computing technical capacities (5.3) w.r.t. the gas transport model (WBF). Entry nodes are indicated by circles, exits by boxes, and inner nodes by diamonds. Lower and upper pressure bounds are denoted by $[\pi^-, \pi^+]$ at the corresponding nodes.

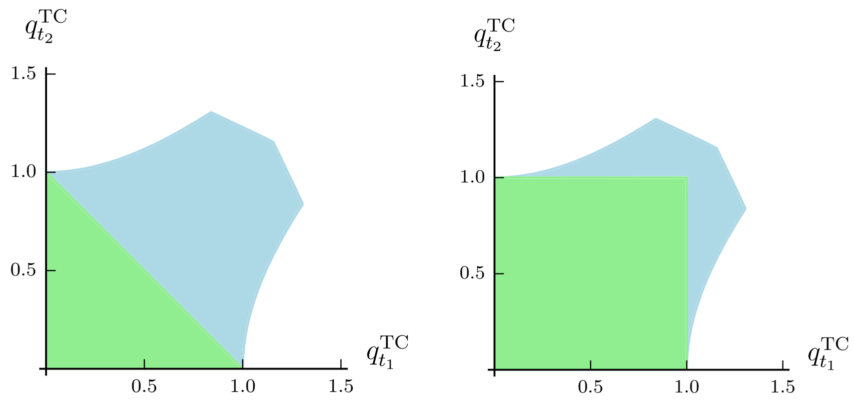

Figure 5.2.: Illustration of the exit loads ℓ_{t_1} and ℓ_{t_2} with $\ell \in N(q^{\mathrm{TC}})$ for feasible technical capacities $q^{\mathrm{TC}} = (q_s^{\mathrm{TC}}, q_v^{\mathrm{TC}}, q_{t_1}^{\mathrm{TC}}, q_{t_2}^{\mathrm{TC}})^T = (1, 0, 1, 1)^T$ (green, left) and for $q^{\mathrm{TC}} = (2, 0, 1, 1)^T$ (green, right) of the instance given by Figure 5.1. The set of all feasible exit loads of F_N is given in blue in the background of both figures.[2]

Concluding this section, we evaluate the role of bookings and technical capacities within the considered market system. To do so, we briefly sketch the basic structure of a multilevel model of the European entry-exit gas market system developed in [64]. For this model perfect competition is assumed, i.e., all agents act as price takers, and the TSO is regulated. Our description follows the one in [64] and [JT8]. We note that the presented four-level structure of the model corresponds to the timing within the considered market organization and is directly derived from the European directive [45] and its subsequent regulation [47]. As outlined in [JT8], the four-levels of the entry-exit gas market system can be summarized as follows

(i) The TSO is obliged to allocate feasible technical capacities and further determines booking price floors to recover the later arising transportation costs.

(ii) The gas traders competitively buy capacity-rights in form of bookings up to the allocated technical capacities.

[2] The set of feasible exit loads can be computed by the approaches in [62, 81]. For similar network instances, the set of feasible nominations is also discussed in e.g., [62, 71, 114].

(iii) The gas traders nominate gas up to the booked capacities at the day-ahead market.

(iv) The TSO transports the nominations through the network at minimum costs.

In line with the goals of the regulation [47], it is assumed that the TSO aims at maximizing the social welfare; see [64] for a complete description of the model. The trading of gas within feasible technical capacities does not directly depend on the corresponding gas transport since it is guaranteed that every balanced load flow within these technical capacities can be transported through the network. Thus, technical capacities decouple trading and transport of gas, which is the main goal of the European entry-exit gas market system. However, decoupling transport and trading of gas may lead to economic inefficiencies. To measure such welfare losses within the considered market system is very challenging and is one of the main goals of the sketched multilevel model [64]. This model can be reformulated as a bilevel problem under mild assumptions as shown in [64], which then can be recast to a single level mixed-integer nonlinear model; see [26] and [JT8]. This single-level reformulation is challenging to solve since it includes the two-stage robust problem of computing feasible technical capacities with the goal to maximize the social welfare. However, using our results of Chapters 6 and 7, it is possible to solve the sketched multilevel model of the European entry-exit gas market [64] for a real-world sized tree-shaped network and nonlinear gas flows; see Section 7.3 and [JT8].

Finally, we note that the uncertainty set $N(q^{\mathrm{TC}})$ of balanced load flows represents demand uncertainties. Thus, our results can also contribute to other potential-based network problems with demand uncertainties; see Section 6.6 for an example.

5.2. Literature Survey: Bookings and Technical Capacities

In this section, we briefly discuss approaches from the literature for deciding the feasibility of a booking (5.2) and computing technical capacities (5.3), which summarizes and extends our corresponding literature reviews in [JT2]–[JT5], [JT7], and [JT8].

First mathematical results regarding bookings are obtained in [107], which provides structural properties for the set of feasible bookings in passive networks and Weymouth based gas transport (WBF). A more comprehensive study on bookings and technical capacities is given in the PhD theses [71, 114]. First results on feasible technical capacities and their relation to robust optimization are discussed in [114]. The author of [71] investigates the problem of computing maximal technical capacities and deciding the feasibility of a booking using semi-algebraic sets and presents an algorithm that solves the considered problems in active networks up to a certain tolerance. The obtained approach is also capable of handling potential-based flows and additionally provides exponential upper bounds for the computational complexity of deciding the feasibility of a booking and computing technical capacities. Moreover, the author of [71] studies the problem of deciding the feasibility of a booking (5.2) for capacitated linear flows (CLF) as gas transport model. In doing so, it is shown that deciding the feasibility of a booking w.r.t. (CLF) is coNP-complete in passive networks in general, but it can be decided in polynomial time for trees.

For potential-based flows, a characterization for the feasibility of a booking in passive networks is obtained in [81], which is also discussed together with our joint results [JT3] and [JT5] regarding bookings in the recently published PhD thesis [90]. Since some of our results are based on the characterization of [81], we review it in detail in Section 6.2. Using this characterization, it is shown in [81] that deciding the feasibility of a booking (5.2) w.r.t. linear potential-based flows, i.e., the potential function in (PBF) is linear, can be done in polynomial time for general networks. Moreover, for simplified linear potential-based flows in passive networks, maximal technical capacities (5.3) can be computed by combining the characterization of [81] and the Karush-Kuhn-Tucker (KKT) approach; see [26]. This is not applicable for accurate nonlinear gas transport models, on which we focus in this dissertation. For nonlinear potential-based flows, deciding the feasibility of a booking can be done in polynomial time for tree-shaped passive networks, see [81], which alternatively follows from our results of [JT7] as explained in Section 6.3.1. This result is also contained in [JT10] under additional assumptions on the potential bounds. If the passive network consists of a single cycle, we show that the feasibility of a booking w.r.t. our nonlinear potential-based flow model (WBF) can also be decided in polynomial time; see [JT3]. We further prove that the latter is coNP-hard for the case of general passive networks; see [JT4]. Switching from deciding the feasibility of a booking to computing maximal technical capacities leads to an even more challenging problem. This is highlighted by our results in [JT7], which show that computing maximal technical capacities is NP-hard for capacitated linear as well as linear and nonlinear potential-based flows. These results hold even on trees. However, it is possible to compute maximal technical capacities w.r.t. nonlinear potential-based flows (WBF) in passive trees using a finite-dimensional convex mixed-integer model as described in [JT8]. In Figure 5.3, we summarize the mentioned results for the computational complexity of deciding the feasibility of a booking and of computing maximal technical capacities in passive networks. For the case of active networks, even deciding the feasibility of a nomination is NP-complete; see [107].

Concluding, we briefly discuss some results of the literature related to bookings and technical capacities. The authors of [51] study the so-called reservation allocation problem for capacitated linear flows, which is closely related to verifying the feasibility of a booking in passive networks. Exploiting the perspective of robust optimization, the authors of [5] develop two approaches for deciding robust feasibility and infeasibility for a specific two-stage robust optimization with empty first stage and additional uniqueness assumption on the second-stage variables. These methods are based on a set containment approach that is then solved by using semidefinite relaxations and are applied to passive gas networks with uncertain pressure drop coefficients. In [4], the authors provide a single-stage reformulation for a problem similar to deciding the feasibility of a booking, in which additionally active elements are present as first-stage variables, i.e., the control of these active elements is decided before the uncertainty reveals itself. This reformulation is then solved by using piecewise linear relaxations and can be used to decide the feasibility of a booking in passive networks. Further, in [80] an adaptive bundle method for nonlinear robust optimization is developed, which is then applied to a more general version of the problem considered in [4]. Unfortunately, these results cannot be used to decide the

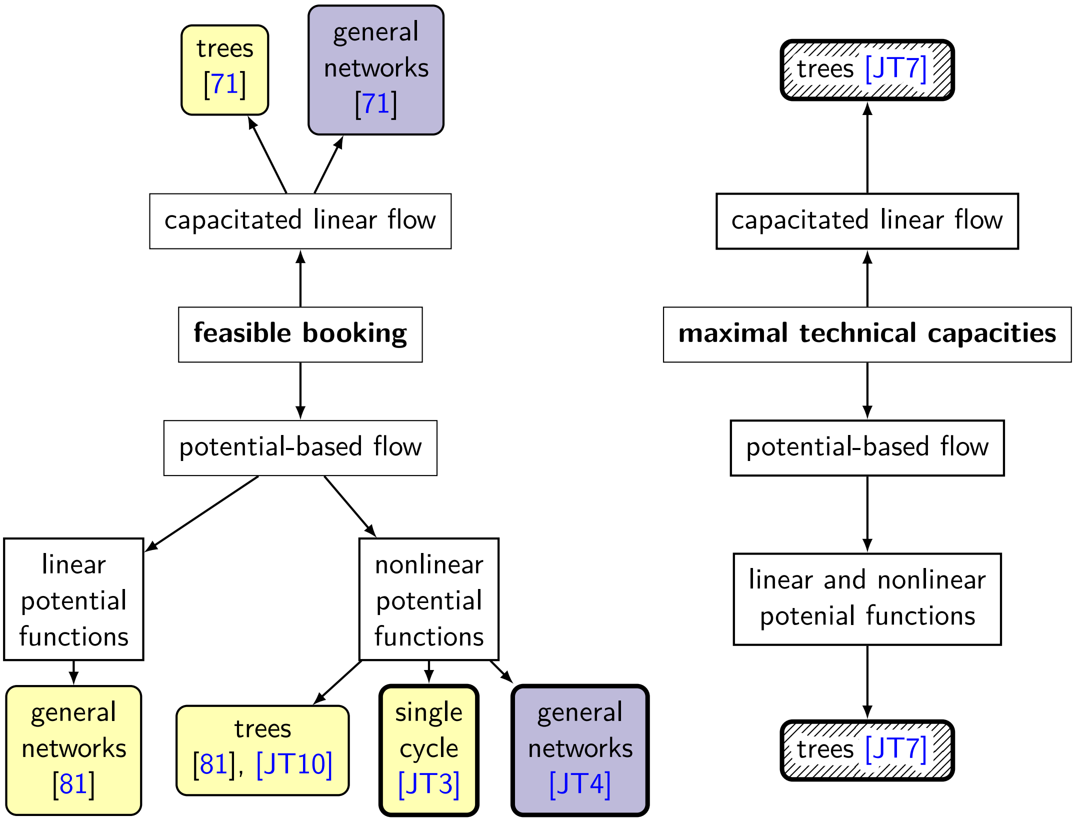

Figure 5.3.: Overview of known complexity results (light=P, dark=coNP-hard, and pattern=NP-hard) for deciding the feasibility of a booking and computing maximal technical capacities in passive networks; adapted and extended version of [JT4, Figure 1] and [81, Figure 3]. We marked the results obtained during the PhD studies by a bold frame.

feasibility of a booking in active networks, which we study in [JT5], since here the control of the active elements can be adjusted after the uncertainty reveals itself, i.e., the control of the active elements is a second-stage decision; see Section 6.5. In [109] a robust treatment of uncertain load flows in passive gas networks is presented, in which the uncertainty affects only exit nodes without any limitation for the supply of entry nodes. For this specific case, the authors provide a reformulation that consists of finitely many scenarios by using monotonicity properties of potential-based flows. Robust network topologies are studied in [76], where robustness is defined by differences of node potentials and their reaction to decreasing demand. The results provide some monotonicity properties of feasible nominations in specific networks. Concluding, we note that many other robust approaches are based on duality concepts and thus, cannot be applied to the considered problems since we focus on nonlinear and nonconvex models of gas transport.

We finally note that also stochastic approaches for potential-based flows under uncertainty related to deciding the feasibility of a booking exist; see e.g., [62, 72]. Further, uncertain loads within the European gas market are addressed in [73] using a joint chance constraint. In [1], a new class of probabilistic/robust so-called “probust” constraints is introduced and applied to gas networks with uncertain load flows.

6. Gas Flows with Load Flow Uncertainties: Deciding Feasibility

In this chapter, we summarize and discuss our results of [JT2]–[JT7] for the problem of deciding the feasibility of a booking (FB). As described in Section 5.1, this problem consists of finding for every balanced load flow below the booking a feasible transport through the network. We focus on our nonlinear potential-based models for gas transport presented in Sections 4.2 and 4.3 and use the notations introduced in Section 5.1. Thus, we adapt the notations of some of the discussed articles. In line with [JT4], the problem of deciding the feasibility of a booking (FB) is given by

Deciding the Feasibility of a Booking (FB).

Input: A weakly connected Graph $G = (V, A)$ with entries V_+, exits V_-, inner nodes V_0, pipes A_{pipe}, active elements A_{act}, a booking $b \in \mathbb{Q}^V_{\geq 0}$, and constraints $c_{\mathcal{E}}(x; \ell) = 0$ and $c_{\mathcal{I}}(x; \ell) \geq 0$.

Question: Is booking b feasible, i.e.,
$\forall \ell \in N(b) = \left\{ \ell \in L \,:\, \ell \leq b, \sum_{u \in V_+} \ell_u = \sum_{u \in V_-} \ell_u \right\}$
$\exists x \in \mathbb{R}^n$ satisfying $c_{\mathcal{E}}(x; \ell) = 0,\ c_{\mathcal{I}}(x; \ell) \geq 0$?

Constraints $c_{\mathcal{E}}(x; \ell) = 0$ and $c_{\mathcal{I}}(x; \ell) \geq 0$ denote one of our models for gas transport of Sections 4.2 and 4.3. Since we study FB also from the perspective of computational complexity, we assume that all constants within the constraints $c_{\mathcal{E}}(x; \ell) = 0$ and $c_{\mathcal{I}}(x; \ell) \geq 0$, e.g., potential bounds $\pi^- \leq \pi^+$, are rational and we use a classical Turing machine as our computational model in the corresponding sections; see [53] for more details on the topic of computational complexity.

In general, our approaches to decide FB are based on exploiting the underlying network structure of graph $G = (V, A)$ together with the additional structure of potential-based flows, given by the link between arc flows and node potentials. The outline of this chapter is as follows. In Section 6.1, we analyze the set of feasible bookings and nominations w.r.t. different models for gas transport. In Section 6.2, we review a characterization for the feasibility of bookings in passive potential-based networks developed in [81]. Based on this characterization, we briefly review results of [81] that allow to decide FB in polynomial time for passive trees and sketch how this result alternatively follows from the ones in [JT7]. Moreover, we discuss our polynomial-time algorithm of [JT3] for deciding FB in passive single-cycle networks in Section 6.3. In the subsequent Section 6.4, we briefly sketch the main ideas of the results of [JT4], which show that deciding FB is coNP-hard in general passive networks. A characterization for the feasibility of bookings w.r.t. nonlinear potential-based flows including linearly modeled active elements (WBFA) is then provided in Section 6.5. Using the results of [JT6] and [JT10], we exemplarily discuss how our results for FB can also be applied to further potential-based network problems with demand uncertainties on the example of computing a robust diameter selection for a tree-shaped hydrogen pipeline network in Section 6.6.

All of the following results originate from our articles [JT2]–[JT7] if not stated otherwise. Throughout this chapter, we also follow the corresponding descriptions of our results within [JT2]–[JT7], to which we refer for more details including all proofs.

6.1. Structural Properties

We now briefly summarize structural properties of FB for different models of gas transport obtained in [JT2]. To do so, we follow the description of the results within [JT2] throughout this section. We analyze if the set of feasible bookings F_B and the set of feasible nominations F_N are bounded, convex, connected, conic, and star-shaped. We note that in [JT2] load flows, nominations, and bookings are defined only for entry and exit nodes, e.g., a load flow is a vector $\ell \in \mathbb{R}_{\geq 0}^{V_+ \cup V_-}$. However, this is no issue w.r.t. our definitions of Section 5.1, in which we include inner nodes, since the corresponding values of the inner nodes are always set to zero.

As in [JT2], we consider the following four different models of gas transport. As preliminary example, we consider a linear flow model consisting only of Kirchhoff's first law (4.3). We further consider our capacitated linear flow model (CLF), which contains additional lower and upper flow bounds. Both models neglect node potentials and for the case of (CLF) checking the feasibility of a nomination $\ell \in N$ is a standard l-transshipment problem; see [103, Chapter 11]. Additionally, we consider our nonlinear potential-based model (WBF) for passive networks with additional arc flow bounds (CLF a). For this model, we assume that the potential bounds satisfy $\cap_{u \in V}[\pi_u^-, \pi_u^+] \neq \emptyset$ since otherwise the set of feasible bookings is empty; see Lemma 4.4 in [JT2]. Our last model, denoted by (NLFA), extends the previous nonlinear potential-based model (WBF) with flow bounds (CLF a) to active networks by adding compressors. In contrast to Section 4.3, we used a nonlinear model for compressors in [JT2]. Since we later focus on our linearly modeled active elements in Section 4.3, we refer to Section 5 of [JT2] for details about the nonlinear compressor model in (NLFA).

We now turn to the analysis of structural properties regarding the set of feasible bookings F_B and the set of feasible nominations F_N, where feasible is meant w.r.t. the previously described models of gas transport. Our results of [JT2] are summarized in Table 6.1 and reveal some rather counter-intuitive properties regarding the set of feasible bookings. For example, the set of feasible bookings is generally nonconvex for all considered models except for the very simplified linear flow model without arc flow bounds. This also indicates that optimizing over this set, i.e., computing maximal technical capacities, is likely to be hard, which we prove in [JT7]; see Section 7.1. The main difference between the linear flow models (4.3) and (CLF) in comparison with the potential-based flow models (WBF),(CLF a) and (NLFA) is that the set of feasible nominations F_N is convex for linear flows, which is not the case for our nonlinear potential-based flow models.

As described in [JT2], the only desirable properties of the set of feasible bookings for the case of active networks directly result from the nature of bookings and are

Table 6.1.: Summary about properties of the set of feasible nominations F_N and the set of feasible bookings F_B w.r.t. different gas transport models; adapted version of [JT2, Table 5] [1].

Properties	Gas transport constraints (4.3)	(CLF)	(WBF),(CLF a)	(NLFA)
Bounded F_N	×	✓	✓	✓
Bounded F_B	×	×	×	×
Convex F_N	✓	✓	×	×
Convex F_B	✓	×	×	×
Connected F_N	✓	✓	✓	×
Connected F_B	✓	✓	✓	✓
Star-shaped F_N	✓	✓	✓	×
Star-shaped F_B	✓	✓	✓	✓
Conic F_N	✓	×	×	×
Conic F_B	✓	×	×	×

independent from the chosen model of gas transport. We finally note that for linearly modeled active elements as in (WBFA) the set of feasible nominations F_N is neither connected nor star-shaped, which follows from Section 3 in [JT5] and is in line with the presented results for (NLFA) in [JT2].

6.2. Review of a Characterization for Feasibility in Passive Networks

We now review a characterization for the feasibility of bookings in passive potential-based networks obtained in [81], which we use in the subsequent Sections 6.3 and 6.4. To be in line with these sections, we explicitly consider our potential-based model (WBF) in the following. However, this characterization is also applicable to our general potential-based flow model (PBF); see [81].

As shown in [81], FB w.r.t. (WBF) can be decided by solving a nonlinear optimization problem for each pair of nodes $(w_1, w_2) \in V^2$. The problem computes the maximum potential difference between w_1 and w_2 within the considered booking b and is given by

$$\varphi_{w_1 w_2}(b) := \max_{\ell,q,\pi} \quad \pi_{w_1} - \pi_{w_2} \tag{6.1a}$$

$$\text{s.t.} \quad \sum_{a\in\delta^{\text{out}}(v)} q_a - \sum_{a\in\delta^{\text{in}}(v)} q_a = \begin{cases} \ell_v, & v \in V_+, \\ -\ell_v, & v \in V_-, \\ 0, & v \in V_0. \end{cases} \tag{6.1b}$$

$$\pi_u - \pi_v = \Lambda_a |q_a| q_a, \quad a = (u,v) \in A, \tag{6.1c}$$

$$0 \le \ell_u \le b_u, \quad u \in V, \tag{6.1d}$$

[1] Adapted by permission from Springer Nature Customer Service Centre GmbH: Springer Nature, 4OR from L. Schewe, M. Schmidt, and J. Thürauf. “Structural properties of feasible bookings in the European entry-exit gas market system”. In: *4OR* 18.2 (2020), pp. 197–218. DOI: 10.1007/s10288-019-00411-3, © Springer-Verlag GmbH Germany, part of Springer Nature 2019. All rights reserved. 2020

where $\Lambda_a > 0$ for $a \in A$ is an arc specific constant and $\varphi_{w_1 w_2}$ is the corresponding optimal value function that denotes the maximum potential difference between nodes w_1 and w_2. The Constraints (6.1b) and (6.1c) equal our Weymouth based model of gas transport (WBF) except that we dismiss potential bounds. Further, Constraints (6.1d) ensures that only booking-compliant nominations are considered. Using the nonlinear optimization problem (6.1), the feasibility of a given booking can be characterized as shown in [81].

Theorem 6.2.1 (Theorem 10 in [81])**.** *Let $G = (V, A)$ be a weakly connected and passive network and $b \in \mathbb{R}^V_{\geq 0}$ be a booking. Then, booking b is feasible w.r.t.* (WBF) *if and only if for each pair of nodes $(w_1, w_2) \in V^2$ the corresponding optimal value $\varphi_{w_1 w_2}(b)$ of* (6.1) *satisfies*

$$\varphi_{w_1 w_2}(b) \leq \pi^+_{w_1} - \pi^-_{w_2}. \tag{6.2}$$

Remark 6.2.2. Characterization (6.2) in Theorem 6.2.1 is also valid for our general potential-based flow model (PBF); see [81]. To this end, we only have to replace Constraints (6.1c) by (PBF a). Arc flow bounds can be integrated as well; see [81].

We note that Theorem 6.2.1 can be seen as a generalization of Theorem 3 in [JT10], which provides a similar characterization for tree-shaped networks under additional assumptions on the potential bounds. We further note that we extend the characterization of Theorem 6.2.1 to the case of active networks with linearly modeled compressors and control valves in [JT5]; see Section 6.5.

From the reviewed characterization, it directly follows that for linear potential-based flows, i.e., the potential functions in (PBF) are linear, FB can be decided in polynomial time; see [81]. However, for the case of capacitated linear flows (CLF), deciding FB is coNP-complete; see [71]. Comparing the results of [81] and [71] shows that exploiting the link between potentials and flows in potential-based networks may lead to efficient solution algorithms if this link is rather simple. However, the coupling between potentials and flows is usually nonlinear; see Section 4.2. In the following sections, we exploit this coupling for nonlinear potential-based flows together with the underlying network structure to derive approaches for deciding FB.

6.3. Polynomial-Time Results for Passive Tree-shaped and Passive Single-Cycle Networks

Using the characterization of Theorem 6.2.1, we now review results of [81] that allow to decide the feasibility of a booking FB in polynomial time for passive trees. In addition, we sketch how this result can also be proven by our results of [JT7] using a slightly different approach. Furthermore, we provide an algorithm that decides the feasibility of a booking in polynomial time for passive single-cycle networks developed in [JT3]. To be consistent with most of our articles, we present our results for our potential-based flow model (WBF) based on the Weymouth equation and explicitly remark to what extent our results are applicable to our general potential-based flow model (PBF).

Since the physical flow in potential-based networks is not influenced by the orientation of the arcs, we use so-called flow-paths throughout this section. These are formally introduced in [JT3] and [JT7] as follows. For nodes $u, v \in V$, a flow-path $P := P(u,v) = (V(u,v), A(u,v))$ contains the nodes of a path from u to v in the undirected version of the graph G, i.e., $V(u,v) \subseteq V$, and $A(u,v) \subseteq A$ contains the corresponding directed arcs of this path. We say that $P(u,v)$ is a directed flow-path from u to v if $P(u,v)$ is a directed path from u to v in graph G. Further, we call a flow-path $P(u',v')$ with $u', v' \in V$ a *flow-subpath* of $P(u,v)$ if $P(u',v') \subseteq P(u,v)$, i.e., $V(u',v') \subseteq V(u,v)$ and $A(u',v') \subseteq A(u,v)$, holds. A flow-path can be seen as undirected path that additionally encodes for each edge its direction in the graph $G = (V, A)$.

6.3.1. Review Results for Tree-shaped Networks

Throughout this section, we assume that graph $G = (V, A)$ is a tree, i.e., the corresponding undirected graph of G does not contain any cycle. We now briefly review results of [81] that allow to decide the feasibility of a booking (FB) in polynomial time in passive trees. In addition, we sketch how this result can alternatively be proven by our results of Section 3.1 in [JT7], which are based on the approach of [JT10]. The latter article [JT10] contains that FB can be decided in polynomial time in passive trees under additional assumptions on the potential bounds.

We first introduce some necessary notations taken from [JT7] and [JT8]. We note that the flow-path between two nodes is unique since graph G is a tree. For a given flow-path $P(u,v) = (V(u,v), A(u,v))$, we partition the arcs into $A^{\rightarrow}(u,v)$ and $A^{\leftarrow}(u,v)$. The set $A^{\rightarrow}(u,v)$ consists of all arcs of the flow-path $P(u,v)$ that are directed from u to v, i.e., an arc $(u',v') \in A^{\rightarrow}(u,v)$ satisfies $P(v',v) \subset P(u',v)$. The set $A^{\leftarrow}(u,v) = A(u,v) \setminus A^{\rightarrow}(u,v)$ consists of the remaining arcs of the flow-path $P(u,v)$. For a given flow-path, this partition of the arcs is unique. We further introduce two sub-graphs depending on a given arc $a = (u,v) \in A$, which we later use to determine the maximal flow on this arc a. If we remove arc $a = (u,v)$ from the graph, then the tree decomposes into two sub-trees. We denote the sub-tree that includes node u by $G_u = (V_u^{(u,v)}, A_u^{(u,v)})$ and the other sub-tree that includes node v by $G_v = (V_v^{(u,v)}, A_v^{(u,v)})$. Thus, $V_v^{(u,v)} = V \setminus V_u^{(u,v)}$ holds.

In [81], Theorem 6.2.1 is applied to decide FB. Thus, for each pair of nodes $(w_1, w_2) \in V^2$, it is necessary to compute the maximum potential difference between w_1 and w_2 within the considered booking b, which is given by the optimal value $\varphi_{w_1 w_2}(b)$ of the nonlinear and nonconvex problem (6.1). This can be done in polynomial time for tree-shaped passive networks, which is formally proven in [81] by using techniques of dynamic programming. To this end, it is shown in [81] that the optimal value function $\varphi_{w_1 w_2}$ can be modeled using tree-specific flow bounds. These flow bounds depend on a given booking and bound the flows corresponding to a booking-compliant nomination in trees as e.g., proven in [JT7].

Lemma 6.3.1 (Lemma 3.2 in [JT7])**.** *Let $G = (V, A)$ be a tree, $b \in \mathbb{R}^V_{\geq 0}$ a booking, $\ell \in N(b)$ a nomination, and q its unique flow given by (6.1b). Then, for every* *arc* $a = (u, v) \in A$, *the flow* q_a *is bounded by*

$$\begin{aligned} \xi_a^-(b) &:= -\min\left\{ \sum_{w \in V_+ \cap V_v^{(u,v)}} b_w, \sum_{w \in V_- \cap V_u^{(u,v)}} b_w \right\} \le q_a, \\ q_a &\le \min\left\{ \sum_{w \in V_+ \cap V_u^{(u,v)}} b_w, \sum_{w \in V_- \cap V_v^{(u,v)}} b_w \right\} =: \xi_a^+(b). \end{aligned} \tag{6.3}$$

As described in [JT7], these bounds state that the maximum arc flow is bounded by the minimum of the aggregated bookings of the entries at one side of the arc and of the aggregated bookings of the exits at the other side of the arc. In a slightly different setting, it is proven in [81] that the flow bounds (6.3) are tight and can be used to express the optimal value function $\varphi_{w_1 w_2}$ as follows.

Corollary 6.3.2 (Corollary 19 in [81]). *Let* $G = (V, A)$ *be a tree,* $b \in \mathbb{R}^V_{\ge 0}$ *a booking, and* $w_1, w_2 \in V$. *Then,*

$$\varphi_{w_1 w_2}(b) = \sum_{a \in A^{\rightarrow}(w_1, w_2)} \Lambda_a \xi_a^+(b)^2 + \sum_{a \in A^{\leftarrow}(w_1, w_2)} \Lambda_a \xi_a^-(b)^2 \tag{6.4}$$

holds, where $\xi_a^+(b)$ *and* $\xi_a^-(b)$ *are the upper and lower arc flow bounds given by* (6.3) *and* $\varphi_{w_1 w_2}$ *is the optimal value function of* (6.1).

For a given booking b, the flow bounds (6.3) can be computed in polynomial time; see e.g., [81]. Thus, from Corollary 6.3.2 and Theorem 6.2.1 it directly follows that the feasibility of a booking w.r.t. (WBF) can be decided in polynomial time in passive trees, which is formally proven for general potential-based flows in Theorem 20 in [81].

Corollary 6.3.3 (Theorem 20 in [81]). *The feasibility of a booking* $b \in \mathbb{Q}^V_{\ge 0}$, *i.e., FB, w.r.t.* (WBF) *can be checked in polynomial time in tree-shaped passive networks.*

We now briefly sketch how this result, especially Corollary 6.3.2 can alternatively be proven by using our results of [JT7], which are based on the approach of [JT10]. As in [81], the main idea is based on the following. For a given pair of nodes $(w_1, w_2) \in V^2$, the potential difference between w_1 and w_2 increases if we send more flow from w_1 to w_2 since for every arc $a \in A$ the potential function $\psi_a(q_a) = \Lambda_a q_a |q_a|$ is strictly increasing w.r.t. the arc flow q_a. Using the network structure of trees, we can efficiently compute booking-compliant nominations for which the flow between w_1 and w_2 is maximal for every arc of the unique flow-path $P(w_1, w_2)$. Consequently, these nominations lead to the maximum potential difference between w_1 and w_2. Moreover, these nominations with maximal arc flow can be computed in polynomial time as proven in [JT7].

Lemma 6.3.4 (Lemmas 3.4 and 3.5 in [JT7]). *Let* $G = (V, A)$ *be a tree,* $b \in \mathbb{R}^V_{\ge 0}$ *a booking, and* $w_1 \neq w_2 \in V$. *Furthermore, let* $P(w_1, w_2)$ *be a directed flow-path from* w_1 *to* w_2. *Then, two nominations* $\ell, \tilde{\ell} \in N(b)$ *with unique flows* q *and* $\tilde{q}$, *satisfying* (6.1b), *exist such that for every arc $a = (u, v) \in A(w_1, w_2)$, the corresponding arc flow is at its upper, respectively lower bound in (6.3), i.e.,*

$$q_a = \xi_a^+(b), \quad \tilde{q}_a = \xi_a^-(b), \tag{6.5}$$

holds for every $a \in A(w_1, w_2)$. Additionally, we can compute these nominations ℓ and $\tilde{\ell}$ in polynomial time.

As discussed in [JT3] and [JT7], we can w.l.o.g. assume that flow-path $P(w_1, w_2)$ is a directed path from w_1 to w_2 in Problem (6.1) since if an arc has an opposite direction, we just switch the sign of the corresponding flow variable.

The maximum potential difference between w_1 and w_2, computed by Problem (6.1), depends on *all* arc flows of the unique flow-path $P(w_1, w_2)$. Thus, the key point of Lemma 6.3.4 is that there exists a nomination with corresponding unique flows so that *all* arc flows of the flow-path $P(w_1, w_2)$ are at the upper, respectively lower, arc flow bound. As direct consequence, it follows that we can express the optimal value function $\varphi_{w_1 w_2}$ of the nonlinear problem (6.1) by the lower and upper arc flow bounds (6.3) as in Corollary 6.3.2. Moreover, we can compute a nomination $\ell \in N(b)$ with maximum flow q satisfying (6.5) in polynomial time by solving a single linear problem that can also be solved by a combinatorial algorithm both developed in [JT10]; see the proofs of Lemmas 3.4 and 3.5 in [JT7] for details. Consequently, this short explanation sketches how our results of [JT7] can also provide an alternative proof for the result that the feasibility of a booking can be decided in polynomial time in passive trees, which is proven in [81] by using techniques of dynamic programming to compute a nomination with maximum flow satisfying (6.5) that induces the maximum potential difference.

Remark 6.3.5. As formally proven in [81], the results of this section are also valid for our general potential-based flow model (PBF) if the potential functions can be evaluated in polynomial time. This is based on the fact that only the monotonicity of the potential difference between w_1 and w_2, i.e., the objective function of (6.1), w.r.t. the flows q is exploited. Further, the nominations with maximum flows, see Lemma 6.3.4, are independent from the potential function and are only based on the tree structure of the network and the flow constraints (6.1b).

6.3.2. Single-Cycle Networks

In general, solving Problem (6.1) for cyclic networks is more difficult than for trees since the potential drop along each cycle has to sum up to zero. Thus, for two flow-paths $P(u, v)$ and $\tilde{P}(u, v)$ and a feasible point (ℓ, q, π) of (6.1), the Constraints (6.1c) implicitly enforce the following equation

$$\begin{aligned} \pi_u - \pi_v &= \sum_{a \in A^{\rightarrow}(u,v)} \Lambda_a q_a |q_a| - \sum_{a \in A^{\leftarrow}(u,v)} \Lambda_a q_a |q_a| \\ &= \sum_{a \in \tilde{A}^{\rightarrow}(u,v)} \Lambda_a q_a |q_a| - \sum_{a \in \tilde{A}^{\leftarrow}(u,v)} \Lambda_a q_a |q_a| , \end{aligned}$$

where $A^{\rightarrow}(u,v)$ consists of all arcs of the flow-path $P(u,v)$ that are directed from u to v and the remaining arcs of $P(u,v)$ are included in $A^{\leftarrow}(u,v)$. In analogy, $\tilde{A}^{\rightarrow}(u,v)$ and $\tilde{A}^{\leftarrow}(u,v)$ are defined for $\tilde{P}(u,v)$. We note that this implicit equation is not relevant in tree-shaped networks since the flow-path is unique for two nodes in trees.

We now turn to the case of a single-cycle network, i.e., the network only consists of a single cycle; see the network in Figure 6.1. Throughout this section, we say that $G=(V,A)$ is a single cycle if the undirected graph underlying G consists of a single cycle. In the following, we discuss the main ideas of our approach of [JT3] that decides FB w.r.t. (WBF) in polynomial time for the case of a single-cycle network. To do so, we closely follow the description of the results within [JT3] throughout this section. For a detailed explanation including all proofs, we refer to [JT3]. In a single-cycle network, for two nodes $u,v \in V$ exactly two different flow-paths connecting u and v exist. As in [JT3], $P^{\mathrm{l}}(u,v)=(V^{\mathrm{l}}(u,v),A^{\mathrm{l}}(u,v))$ represents the *left path*, which is obtained when v is reached in counter-clockwise direction from u, and $P^{\mathrm{r}}(u,v)=(V^{\mathrm{r}}(u,v),A^{\mathrm{r}}(u,v))$ represents the *right path*, which is obtained by using the clockwise direction. This leads to the following partition of the arcs $A=A^{\mathrm{l}}(u,v)\cup A^{\mathrm{r}}(u,v)$.

As in the previous section, we characterize the feasibility of a booking by Theorem 6.2.1. Thus, a given booking b is feasible if and only if for every pair of nodes $(w_1,w_2)\in V^2$ the constraint system

$$\pi_{w_1}-\pi_{w_2}>\pi^{+}_{w_1}-\pi^{-}_{w_2}, \quad (6.1b)\text{–}(6.1d), \tag{6.6}$$

admits no solution. Our approach of [JT3] is based on the following idea. We exploit properties of single-cycle networks and potential-based flows that enable us to reduce (6.6) to a system of polynomials of constant dimension independent from the size of the considered cycle. We then apply tools from real algebraic geometry to this system of fixed dimension in order to obtain a polynomial-time algorithm for deciding FB w.r.t. (WBF).

An important property of potential-based flows in passive networks is that there cannot be any cycling flow as outlined in [68]. Consequently, in a single-cycle network flow from different directions has to "meet" in at least one node, which are introduced in [JT3] as so-called flow-meeting points.

Definition 6.3.1. Let $G=(V,A)$ be a single cycle. Let further (ℓ,q,π) satisfy (6.1b) and (6.1c) with $\ell\in N\setminus\{0\}$ and let $o\in V_+$ be an entry node with highest potential, i.e., $\pi_o\geq\pi_v$ for all $v\in V$. Then, $w\in V\setminus\{o\}$ is a *flow-meeting point* if there exist $u\in V^{\mathrm{l}}(o,w)$ adjacent to w that satisfies $\pi_u>\pi_w$ as well as $v\in V^{\mathrm{r}}(o,w)$ such that $\pi_v>\pi_w$ and $\pi_{v'}=\pi_w$ holds for all $v'\in V^{\mathrm{r}}(v,w)\setminus\{v\}$.

An illustrative example for this definition is given in Figure 6.1, which also shows that there can be multiple flow-meeting points for a feasible point of (6.1). However, exploiting that for every $a\in A$ the considered potential function $\psi_a(q_a)=\Lambda_a q_a|q_a|$ is strictly increasing w.r.t. the arc flow q_a, we prove in [JT3] that there always is an optimal solution of the nonlinear problem (6.1) with at most one flow-meeting point.

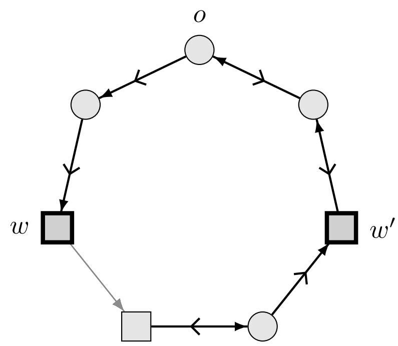

Figure 6.1.: Flow directions and resulting flow-meeting points. Entry nodes are indicated by circles and exit nodes by boxes. Bold arcs indicate flow directions, whereas gray arcs indicate zero arc-flow. In this example, exit nodes w and w' are flow-meeting points and o is an entry node with highest potential level; adapted version of [JT3, Figure 2; licensed under CC BY 4.0].

Theorem 6.3.6 (Theorem 12 in [JT3])**.** *Let $G = (V, A)$ be a single cycle, b be a booking, and $(w_1, w_2) \in V^2$ be a fixed pair of nodes. Then, there is an optimal solution of Problem (6.1) that has at most one flow-meeting point w.*

Using this result, we prove in [JT3] that we can reduce the search space of Problem (6.1) by enforcing nonnegative flows.

Corollary 6.3.7 (Corollary 13 in [JT3])**.** *Let $G = (V, A)$ be a single cycle, b be a booking, and $(w_1, w_2) \in V^2$ be a fixed pair of nodes. Then, there exist nodes $(o, w) \in V_+ \times V_-$ and an optimal solution (ℓ, q, π) of Problem (6.1) with $q \geq 0$, if we assume that $P^l(o, w)$ and $P^r(o, w)$ are directed paths from o to w.*

As described in [JT3], this result allows us to focus on the following variant of Problem (6.1) for every pair of nodes $(o, w) \in V_+ \times V_-$

$$\bar{\varphi}^{ow}_{w_1 w_2}(b) := \max_{\ell, q, \pi} \ \pi_{w_1} - \pi_{w_2}, \quad \text{s.t. (6.1b)–(6.1d)}, \ q_a \geq 0, \ a \in A, \tag{6.7}$$

where the arcs A are oriented from o to w. Moreover, a given booking b is feasible if and only if for every pair of nodes $(w_1, w_2) \in V^2$ and $(o, w) \in V_+ \times V_-$ the constraint system

$$\pi_{w_1} - \pi_{w_2} > \pi^+_{w_1} - \pi^-_{w_2}, \quad \text{(6.1b)–(6.1d)}, \ q_a \geq 0, \ a \in A, \tag{6.8}$$

admits no solution, where the arcs A are oriented from o to w; see Corollary 15 in [JT3].

Exploiting properties of potential-based flows and of the single-cycle network, we prove in Section 5 of [JT3] that there always is an optimal solution (ℓ, q, π) of Problem (6.7) in which the nomination ℓ satisfies specific properties. These enable us to reduce (6.8) to a system of polynomials with fixed number of constraints and variables independent from the size of the cycle. Since the proven properties depend on the location of w_1 and w_2, we present an exemplary case in this extended summary, namely $w_1, w_2 \in V^{\mathrm{r}}_+(o, w)$, on the basis of which the polynomial-time algorithm is presented in Section 6 of [JT3].

Theorem 6.3.8 (Theorem 35 in [JT3])**.** *Let $G = (V, A)$ be a single cycle. Further, let $(o, w) \in V_+ \times V_-$ be fixed and $w_1, w_2 \in P^r(o, w)$. Then, an optimal solution (ℓ, q, π) of Problem (6.7) exists that satisfies*

(a) Two entries $s^l_1, s^l_2 \in V^l_+(o, w)$ with $P^l(o, s^l_1) \subseteq P^l(o, s^l_2)$ exist such that

$$\begin{aligned} \ell_v &= 0, \quad v \in \left(V^l_+(o, s^l_1) \cup V^l_+(s^l_2, w)\right) \setminus \left\{o, s^l_1, s^l_2\right\}, \\ \ell_v &= b_v, \quad v \in V^l_+(s^l_1, s^l_2) \setminus \left\{s^l_1, s^l_2\right\}. \end{aligned}$$

(b) An exit $t^l_1 \in V^l_-(o, w)$ exists such that

$$\begin{aligned} \ell_v &= 0, \quad v \in V^l_-(o, t^l_1) \setminus \left\{t^l_1\right\}, \\ \ell_v &= b_v, \quad v \in V^l_-(t^l_1, w) \setminus \left\{t^l_1\right\}. \end{aligned}$$

(c) Two entries $s^r_1, s^r_2 \in V^r_+(o, w)$ with $P^r(o, s^r_1) \subseteq P^r(o, s^r_2)$ exists such that

$$\begin{aligned} \ell_v &= 0, \quad v \in \left(V^r_+(o, s^r_1) \cup V^r_+(s^r_2, w)\right) \setminus \left\{o, s^r_1, s^r_2\right\}, \\ \ell_v &= b_v, \quad v \in V^r_+(s^r_1, s^r_2) \setminus \left\{s^r_1, s^r_2\right\}, \end{aligned}$$

(d) Two exits $t^r_1, t^r_2 \in V^r_-(o, w)$ with $P^r(o, t^r_1) \subseteq P^r(o, t^r_2)$ exist such that

$$\begin{aligned} \ell_v &= 0, \quad v \in \left(V^r_-(o, t^r_1) \cup V^r_-(t^r_2, w)\right) \setminus \left\{t^r_1, t^r_2, w\right\}, \\ \ell_v &= b_v, \quad v \in V^r_-(t^r_1, t^r_2) \setminus \left\{t^r_1, t^r_2\right\}. \end{aligned}$$

An exemplary optimal solution of Problem (6.7) satisfying Properties (a)–(d) is illustrated in Figure 6.2. From Theorem 6.3.8 it follows that after determining the nodes $o, w, s^l_1, s^l_2, t^l_1, s^r_1, s^r_2, t^r_1, t^r_2$, we can directly assign the values of the nomination ℓ of the remaining nodes in an optimal solution of Problem (6.7) by (a)–(d). This holds analogously for the case $w_1, w_2 \in P^{\mathrm{l}}(o, w)$ and a similar result for Theorem 6.3.8 is proven for the case that $w_1, w_2 \in V$ lie on opposite sides of the cycle, e.g., $w_1 \in P^{\mathrm{l}}(o, w)$ and $w_2 \in P^{\mathrm{r}}(o, w)$; see Section 5 of [JT3].

As described in [JT3], we can exploit our obtained properties of specific optimal solutions of Problem (6.7), e.g., given by Theorem 6.3.8, to reduce System (6.8) to a system of polynomials in fixed dimension independent from the size of the cycle.

Theorem 6.3.9 (Theorem 39 in [JT3])**.** *Let $G = (V, A)$ be a single cycle. System (6.8) can be reduced in polynomial time to a system of polynomials with at most 9 variables and 42 constraints.*

As discussed in [JT3], we can now apply a general decision algorithm for the existence of solutions of a system of polynomials, see Algorithm 14.16 in [9], to decide in polynomial time if our reduced system of polynomials with fixed number of variables and constraints admits a solution or not; see Theorem 40 in [JT3]. Applying this procedure to all pairs of nodes $(o, w) \in V_+ \times V_-$ and exploiting the presented properties of specific optimal solutions lead to the final result that deciding FB w.r.t. the nonlinear gas transport model (WBF) can be done in polynomial time in a single-cycle network as outlined in Section 6 of [JT3].

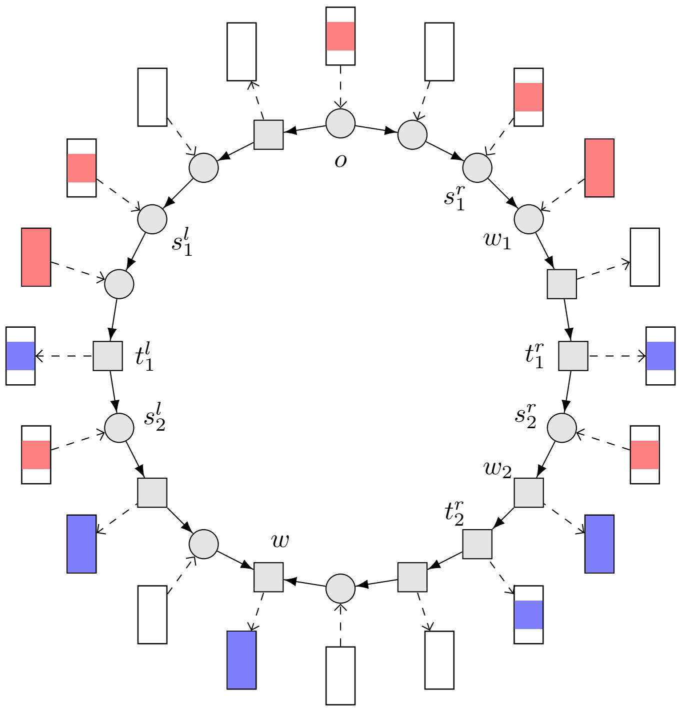

Figure 6.2.: Exemplarily configuration of s and t nodes with $w_1, w_2 \in P^r(o, w)$ satisfying Properties (a)–(d). Entry nodes are illustrated by circles and gray boxes illustrate exit nodes. The amount of bookings is qualitatively illustrated by boxes that are attached to the corresponding nodes by dashed arcs; adapted version of [JT3, Figure 4; licensed under CC BY 4.0].

Corollary 6.3.10 (Corollary 41 in [JT3])**.** *The feasibility of a booking $b \in \mathbb{Q}^V_{\geq 0}$, i.e., FB w.r.t. (WBF), can be checked in polynomial time on a cycle.*

Remark 6.3.11. The specific properties of an optimal solution of Problem (6.1) such as Theorem 6.3.8 are also valid for our general potential-based flow model (PBF). However, the presented complexity result is only valid if the potential function $\psi_a(q_a)$ is a polynomial in the variables q_a and $|q_a|$ and satisfies Definition 4.2.3.

Concluding, we remark that our approach does not compute an optimal solution of Problem (6.1). It only decides if a solution of Problem (6.1) with an objective value of at least a specific threshold value exists. This is an important point since for a rational nomination and rational input data the corresponding flows satisfying (WBF) may be irrational, which is exemplarily outlined in Example 4.3 in [90].

For our study regarding the feasibility of a booking, we now proceed from a single-cycle network to general passive networks in the next section.

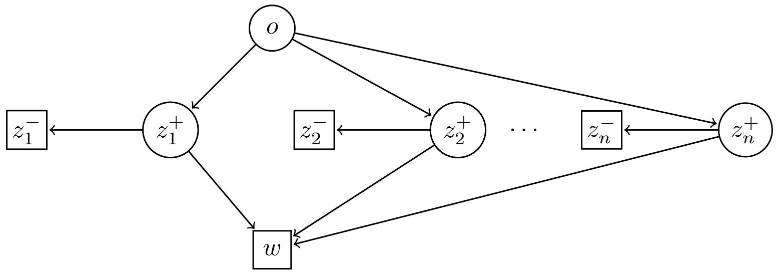

Figure 6.3.: The graph $G(\mathsf{Part})$. Entry nodes are indicated by circles and exit nodes by boxes; adapted version of [JT4, Figure 2].

6.4. coNP-hardness for General Passive Networks

In this section, we briefly discuss the results of [JT4], which prove that deciding FB w.r.t. (WBF) is coNP-hard in general graphs. This result draws the first line that separates the easy from the hard variants of deciding FB for the case of potential-based flows. Since the hardness proof is very technical, we only sketch its main idea following the descriptions within [JT4]. For a complete explanation including all proofs, we refer to [JT4].

As in the previous sections, we characterize the feasibility of bookings w.r.t. (WBF) by computing maximum potential differences; see Theorem 6.2.1. In [JT4], it is proven that FB w.r.t. (WBF) is coNP-hard by reducing the Partition problem to the infeasibility of a booking. We consider Partition with the small adaption of $n \geq 3$, which is still NP-hard; see [53].

Partition (Part).
Input: $S_1, \ldots, S_n \in \mathbb{N}$ with $n \geq 3$, $I = \{1, \ldots, n\}$, and $\sum_{i \in I} S_i = K$.
Question: Does $I_1 \subseteq I$ with $\sum_{i \in I_1} S_i = \sum_{I \setminus I_1} S_i$ exist?

For a given Partition instance, we now sketch the construction of the graph $G(\mathsf{Part}) = (V, A)$ following [JT4]. On the basis of this graph, we then describe the key points of the hardness proof for FB obtained in [JT4].

For each number S_i of the considered Partition instance, the graph $G(\mathsf{Part})$ contains an entry node z_i^+ and an exit node z_i^-, which are connected by an arc. Moreover, we introduce a main entry node o as well as a main exit node w and both nodes are connected to every entry node z_i^+ for $i \in I$. An illustration of the graph $G(\mathsf{Part})$ is given in Figure 6.3. For the constructed graph $G(\mathsf{Part})$, we further consider the following booking b

$$b_o = b_w = \frac{K}{2}, \quad b_{z_i^+} = b_{z_i^-} = S_i, \quad i \in I.$$

The complete description of the instance $G(\mathsf{Part})$ including the lower and upper potential bounds and the potential drop coefficients is given in [JT4]. In the following, we further denote a problem-specific threshold value by $T(K) < 1$, which is formally defined in Section 4 of [JT4].

The booking instance is constructed so that deciding the feasibility of booking b in $G(\mathsf{Part})$ reduces to computing the maximum potential difference $\varphi_{ow}(b)$ between o and w, i.e., solving Problem (6.1) w.r.t. (o, w), booking b, and $G(\mathsf{Part})$.

Corollary 6.4.1 (Corollary 4.2 in [JT4]). *Booking b is feasible for $G(\mathsf{Part})$ if and only if $\varphi_{ow}(b) \leq T(K)$.*

Using several technical results, it is proven in [JT4] that the maximum potential difference between o and w within the booking b in $G(\mathsf{Part})$ given by $\varphi_{ow}(b)$ exceeds the threshold $T(K)$ if and only if the given Partition instance is feasible.

Lemma 6.4.2 (Lemma 4.17 in [JT4]). *The Partition instance is feasible if and only if $\varphi_{ow}(b) > T(K)$ is satisfied in $G(\mathsf{Part})$.*

From this result and Corollary 6.4.1, coNP-hardness of deciding the feasibility of a booking w.r.t. (WBF) follows.

Theorem 6.4.3 (Theorem 4.19 in [JT4]). *Deciding the feasibility of a booking, i.e., FB w.r.t. (WBF), is coNP-hard.*

To conclude this section, we repeat the description within [JT4] regarding the main reasons why the maximum potential difference between o and w in $G(\mathsf{Part})$ exceeds the threshold $T(K)$ if and only if Partition is feasible. To do so, we focus on the case of nonnegative flows, i.e., we additionally require $q \geq 0$ in Problem (6.1), from which then follows the arbitrary case; see [JT4]. Consequently, for every $i \in I$ and solution (ℓ, q, π) of Problem (6.1), we can represent the maximum potential difference $\varphi_{ow}(b)$ by

$$\varphi_{ow}(b) = \pi_o - \pi_w = \Lambda_{(o,z_i^+)} q^2_{(o,z_i^+)} + \Lambda_{(z_i^+,w)} q^2_{(z_i^+,w)}. \tag{6.9}$$

The main idea of the proof is based on the following observation.

Observation 6.4.4 (Observation 4.4 in [JT4]). *Let be $a > 0$ and $b > 0$ with $a^2 + b^2 = c$. Then, $a + b > \sqrt{c}$ holds.*

As described in [JT4], this observation and Equations (6.9) imply that *strictly more* flow $q_{(o,z_i^+)} + q_{(z_i^+,w)}$ is necessary to obtain a specific potential difference $\pi_o - \pi_w$ if $q_{(o,z_i^+)} > 0$ and $q_{(z_i^+,w)} > 0$ hold compared to the case where at least one of these flows is zero. In Lemma 4.6 in [JT4], it is proven that if Partition is infeasible, then in an optimal solution of Problem (6.1) w.r.t. (o, w) there is at least one $i \in I$ so that the strict inequalities $q_{(o,z_i^+)} > 0$ and $q_{(z_i^+,w)} > 0$ hold. However, this is not necessarily the case if Partition is feasible; see Lemma 4.3 and its proof in [JT4]. Thus, *strictly more* flow is necessary to obtain a specific objective value $\varphi_{ow}(b)$ if Partition is infeasible compared to the case if Partition is feasible. This is one of the main reasons why $\varphi_{ow}(b)$ only exceeds the threshold $T(K)$ if Partition is feasible since the total amount of flow is limited by the booking.

After our extensive analysis of deciding the feasibility of a booking in passive networks, we now move on to the case of active elements within the network.

6.5. Characterization for Feasibility in Active Networks

In this section, we discuss our results of [JT5], which provide first steps towards deciding the feasibility of a booking FB w.r.t. nonlinear gas transport with linearly modeled compressors and control valves. Thus, we consider (WBFA) as our model for gas transport throughout this section. In the following, we focus on highlighting our bilevel model to decide FB w.r.t. (WBFA) and exemplarily sketch one of our corresponding solution approaches. To this end, we closely follow the description of our results within [JT5], to which we refer for a complete overview of our results including all proofs.

Unfortunately, the results for deciding FB in passive networks based on the characterization in Theorem 6.2.1 cannot be directly applied to decide FB in active networks, which is demonstrated in Section 3 of [JT5]. One of the reasons for this is that active elements in the network, e.g., compressors and control valves, generally lead to additional binary decisions for switching the active elements on or off. These binary decisions are determined individually for each booking-compliant nomination since the transmission system operator (TSO) can adjust the control of the active elements. From a robust optimization perspective, these binary decisions are adjustable integer variables, which are decided after the load flow uncertainty materializes.

As described in [JT5], we address FB w.r.t. (WBFA) using bilevel optimization techniques based on the following bilevel structure. For a given booking b, the upper-level player aims at finding a booking-compliant nomination that cannot be transported through the network. We refer to this nomination as "worst-case" nomination since it represents the most challenging booking-compliant nomination to be transported by the TSO. The lower-level player represents the TSO that tries to transport this "worst-case" nomination of the upper-level player by controlling the active elements. Consequently, if the TSO can transport every "worst-case" nomination of the upper-level player through the network, then the booking is feasible. Otherwise, it is infeasible. For a general introduction to bilevel optimization, we refer to the books [8, 40] and the recent survey article [75].

As shown in [JT5], we can exploit the sketched bilevel structure to decide FB w.r.t. (WBFA) by solving a bilevel optimization problem.

Proposition 6.5.1 (Proposition 4.1 in [JT5])**.** *Let $G = (V, A)$ be a weakly connected network with linearly modeled active elements $A_{\mathrm{act}} \subseteq A$. Then, the booking $b \in L$ is feasible w.r.t.* (WBFA) *if and only if the optimal value of*

$$\sup_{\ell \in N(b)} \min_{q,\pi,\Delta,y,z} \quad y + z \tag{6.10a}$$

$$\text{s.t.} \quad \text{(WBFA a)–(WBFA c), (WBFA e)},$$

$$\pi_u + y \geq \pi_u^-, \quad u \in V, \tag{6.10b}$$

$$\pi_u - z \leq \pi_u^+, \quad u \in V. \tag{6.10c}$$

is nonpositive.

In Problem (6.10), the upper-level player chooses a "worst-case" booking-compliant nomination with the goal to obtain a maximal violation of the potential bounds measured by $y+z$. Contrarily, the TSO tries to transport the upper-level "worst-case" nomination without violating the potential bounds in the lower level. As discussed in [78], the optimal solution of a bilevel problem is not necessarily attained. However, under the additional Assumption 4 on the location of the active elements, it follows from Theorem 6.5.3 that an optimal solution of Problem (6.10) is attained.

In general, Problem (6.10) is a very challenging bilevel problem since its lower level is nonlinear and nonconvex. For our solution approaches regarding Problem (6.10), we need to impose the following assumption, which is also used in [3, 4].

Assumption 4. *No active element is part of an undirected cycle in G.*

This assumption is a simplification of reality since active elements can appear in cycles, see [102], which then allow different routes for the flow of a given nomination in the network. We note that even if we exclude the possibility of cyclic flows, the flow of a given nomination is not necessarily unique in an active network since it depends on the control of the active elements that can be adjusted differently for a nomination. However, under Assumption 4, the flow corresponding to a given nomination is unique in the considered active network as it is for passive networks, which we exploit in our approaches. We note that the case of general active networks is out of scope of this dissertation, but poses an interesting field for future research.

Theorem 6.5.2 (Theorem 4.2 in [JT5])**.** *Let $G = (V, A)$ be a weakly connected network and suppose that Assumption 4 holds. Then, for a given nomination $\ell \in N$, every feasible point (q, π) of (4.3) and* (WBFA a) *admits the same unique flows q_a for all $a \in A$ and the same unique potential differences $\pi_u - \pi_v$ for all $(u, v) \in A_{\mathrm{pipe}}$.*

This uniqueness result implies that for a given nomination most of the lower-level decisions in Problem (6.10) are predetermined by physics. Consequently, we can reduce the lower-level problem to only contain decisions that are not already fixed by physics. To this end, we consider the so-called *reduced network* $\tilde{G} = (\mathcal{G}, A_{\mathrm{act}})$ as introduced in [94, 95]. The node set $\mathcal{G} := \left\{G_0, G_1, \dots, G_{|A_{\mathrm{act}}|}\right\}$ corresponds to the set of passive subnetworks obtained after removing all active elements $a \in A_{\mathrm{act}}$ from G. Moreover, we denote an active arc $a \in A_{\mathrm{act}}$ alternatively by $a = (G_i, G_j)$ if $a = (u, v)$ with $u \in V(G_i)$ and $v \in V(G_j)$ holds. Figure 6.4 visualizes a network that satisfies Assumption 4 and its corresponding reduced network. We note that the reduced network $\tilde{G}$ is always a tree under Assumption 4.

Using the reduced network and Theorem 6.5.2, it is shown in [JT5] that we can equivalently reformulate Problem (6.10) so that the decisions of the lower-level predetermined by physics are moved to the upper level. As described in [JT5], the upper-level player now chooses the "worst-case" nomination and additionally determines the corresponding flows and potential differences on the pipes predetermined by physics. In doing so, all active elements are inactive, i.e., $\pi_u = \pi_v$ for all $(u, v) \in A_{\mathrm{act}}$. The lower-level player, namely the TSO, then only controls the active elements together with a constant shift of the potentials of every passive subnetwork $G_j \in \mathcal{G}$ to

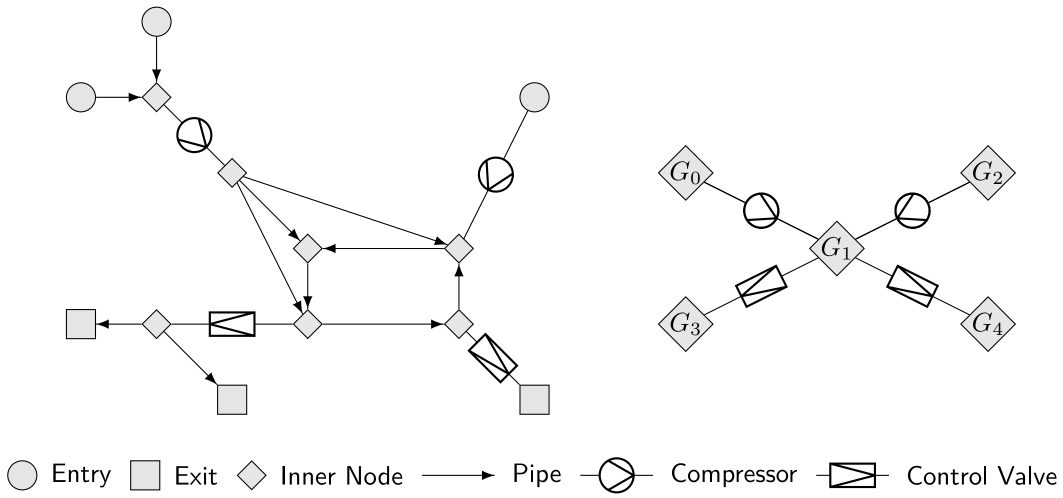

Figure 6.4.: Stylized gas network satisfying Assumption 4 (left) and its reduced network (right); adapted version of [JT5, Figure 2; licensed under CC BY 4.0].

transport the "worst-case" nomination. Thus, the lower level only contains decisions which can actively be determined by the TSO. The obtained bilevel reformulation also enables us to linearly model the indicator function χ_a, which switches active elements on or off in (WBFA), by additional binary variables s_a for $a \in A_{\text{act}}$.

Theorem 6.5.3 (Theorem 4.3 in [JT5]). *Consider the bilevel problem*

$$\max_{\ell,q,\pi,s} \quad y + z \tag{6.11a}$$

$$\text{s.t.} \quad (4.3), (\text{WBFA a}), \ell \in N(b), \tag{6.11b}$$

$$\pi_u = \pi_v, \quad (u,v) \in A_{\text{act}}, \tag{6.11c}$$

$$q_a \leq m_a(1 - s_a) + M s_a, \quad a \in A_{\text{act}}, \tag{6.11d}$$

$$s_a \in \{0,1\}, \quad a \in A_{\text{act}}, \tag{6.11e}$$

$$(\Delta, \tau, y, z) \in \mathcal{R}(\ell, q, \pi, s), \tag{6.11f}$$

where $M := \min\{\sum_{u \in V_+} b_u, \sum_{u \in V_-} b_u\}$ is an upper bound on the flow on any arc and the set of lower-level solutions $\mathcal{R}(\ell, q, \pi, s)$ is given by

$$\arg\min_{\Delta,\tau,y,z} \quad y + z \tag{6.12a}$$

$$\text{s.t.} \quad \tau_i - \tau_j = \begin{cases} -\Delta_a, & a = (G_i, G_j) \in A_{\text{cm}}, \\ \Delta_a, & a = (G_i, G_j) \in A_{\text{cv}}, \end{cases} \tag{6.12b}$$

$$\Delta_a \in [0, \Delta_a^+ s_a], \quad a \in A_{\text{act}}, \tag{6.12c}$$

$$\tau_j + y \geq \pi_u^- - \pi_u, \quad u \in V(G_j),\ G_j \in \mathcal{G}, \tag{6.12d}$$

$$\tau_j - z \leq \pi_u^+ - \pi_u, \quad u \in V(G_j),\ G_j \in \mathcal{G}. \tag{6.12e}$$

Under Assumption 4, Problems (6.10) and (6.11) admit the same optimal value.

The reformulated bilevel problem (6.11) consists of a mixed-integer nonlinear upper level, but the lower level is now a linear problem for fixed upper-level decisions. Consequently, the KKT conditions of the lower level are both necessary and sufficient; see e.g., [27]. A single-level reformulation of Problem (6.11) using the KKT approach is obtained in Section 5 of [JT5], to which we refer for more details on this approach.

In this summary, we focus on an alternative to the KKT reformulation also derived in [JT5], which is based on the lower level's optimal value function; see e.g., [40]. To this end, let $\varphi(\ell, q, \pi, s)$ be the optimal value of (6.12) for given upper-level decisions (ℓ, q, π, s). Since the lower level (6.12) is feasible for every upper-level decisions (ℓ, q, π, s), Problem (6.11) is equivalent to the following single-level reformulation

$$\max_{\ell,q,\pi,s} \{\varphi(\ell, q, \pi, s) \,:\, \text{(6.11b)–(6.11e)}\}\,. \tag{6.13}$$

Since strong duality holds for the lower level, φ is also the optimal value function of the lower level's dual problem. In Section 6 of [JT5], we prove that the optimal value function φ can be represented using polynomially many vertices of the polyhedral feasible set of the lower level's dual problem. Moreover, we explicitly determine these polynomially many vertices in Theorem 6.2 in [JT5]. This is quite surprising since the feasible set of a lower level's dual problem can have exponentially many vertices in general.

To state our closed-form expression for the lower-level optimal value function, we introduce the following notations w.r.t. the reduced network $\tilde{G}$ taken from [JT5]. For a fixed reference node G_k as root of the tree-shaped reduced network $\tilde{G}$, we can partition the active elements into arcs that are directed away from or towards G_k as follows

$$A_{\text{act}}^{k,\rightarrow} := \{(G_i, G_j) \in A_{\text{act}} \,:\, P(G_k, G_i) \subseteq P(G_k, G_j)\}\,, \quad A_{\text{act}}^{k,\leftarrow} := A_{\text{act}} \setminus A_{\text{act}}^{k,\rightarrow}.$$

Analogously, we can partition the set of compressors $A_{\text{cm}} = A_{\text{cm}}^{k,\rightarrow} \cup A_{\text{cm}}^{k,\leftarrow}$ and the set of control valves $A_{\text{cv}} = A_{\text{cv}}^{k,\rightarrow} \cup A_{\text{cv}}^{k,\leftarrow}$. This enables us to present the following closed form of the lower-level optimal value function.

Corollary 6.5.4 (Corollary 6.3 in [JT5])**.** *The optimal value function φ of (6.12) is given by*

$$\max_{\substack{(G_{j_1}, G_{j_2}) \in \mathcal{G}^2,\\ w_1 \in V(G_{j_1}),\\ w_2 \in V(G_{j_2})}} \left\{ \pi_{w_1} - \pi_{w_2} - \left(\pi_{w_1}^{+} - \pi_{w_2}^{-} + \sum_{\substack{a \in P(G_{j_1}, G_{j_2}):\\ a \in A_{\text{cm}}^{j_1,\rightarrow} \cup A_{\text{cv}}^{j_1,\leftarrow}}} \Delta_a^{+} s_a \right) \right\}. \tag{6.14}$$

Consequently, we can decide FB w.r.t. (WBFA) by solving the optimal-value-function reformulation (6.13) in which φ is given by (6.14). This corresponds to optimizing a piecewise-linear function with $|V|^2$ pieces w.r.t. a nonlinear and nonconvex feasible region.

We further derive a characterization of feasible bookings w.r.t. (WBFA), which extends the one given by Theorem 6.2.1 of [81] from passive to active networks.

Similarly to the passive case, we have to compute for each pair of nodes $(w_1, w_2) \in V$ the maximum potential difference between w_1 and w_2. But in active networks, we additionally take into account the control of the active elements, which are adjusted by the TSO to provide a feasible gas transport.

Theorem 6.5.5 (Theorem 6.4 in [JT5]). *Let $G = (V, A)$ be a weakly connected network satisfying Assumption 4. Then, the booking $b \in L$ is feasible if and only if $\phi_{w_1 w_2}(b) \leq \pi_{w_1}^+ - \pi_{w_2}^-$ is satisfied for every pair of nodes $(w_1, w_2) \in V^2$ with $w_1 \in V(G_{j_1})$ and $w_2 \in V(G_{j_2})$, where we define*

$$\phi_{w_1 w_2}(b) := \max_{\ell,q,\pi,s} \left\{ \pi_{w_1} - \pi_{w_2} - \sum_{\substack{a \in P(G_{j_1}, G_{j_2}):\\ a \in A_{\mathrm{cm}}^{j_1,\to} \cup A_{\mathrm{cv}}^{j_1,\leftarrow}}} \Delta_a^+ s_a \colon (6.11\mathrm{b})\text{–}(6.11\mathrm{e}) \right\}.$$

From this characterization it follows that we can decide FB w.r.t. (WBFA) by individually solving $|V|^2$ many mixed-integer nonlinear optimization problems.

Based on the previous results, we develop two similar closed-form expressions of the optimal value function φ and corresponding characterizations for the feasibility of FB w.r.t. (WBFA) in [JT5]. In general, these alternatives consist of less but more challenging subproblems that have to be considered compared to the approach of Corollary 6.5.4 and Theorem 6.5.5. For a description of these approaches, we refer to Section 6.2 and 6.3 of [JT5].

In Section 7 of [JT5], we evaluate the performance of the KKT approach, our optimal-value-function reformulations, and the corresponding characterizations on the basis of GasLib-40 and GasLib-134 of the GasLib [102] for different bookings. In this extended summary, we only briefly state the main conclusions of this computational study and we refer to Section 7 of [JT5] for more details.

Overall, the numerical results indicate that the nonlinear gas transport model (WBFA) is computationally very challenging. Unfortunately, the solvers do not provide consistent results for the considered instances; see Section 7.3 in [JT5]. Thus, we also performed a computational study for simplified linear potential-based flows, i.e., we replaced the right-hand side in (WBFA a) by $\tilde{\Lambda}_a q_a$ with an arc-specific constant $\tilde{\Lambda}_a > 0$; see Section 7.4 in [JT5]. As described in [JT5], the results for the case of linear potential-based flows can be summarized as follows. The KKT approach is already a well-performing approach to decide FB w.r.t. (WBFA). Our approaches based on optimal-value-function reformulations can sometimes outperform the KKT approach. This is especially the case when parallel computing resources are available since then the subproblems of the characterizations can be solved in parallel. The number of binary variables and subproblems in our approaches based on the optimal-value-function reformulations depend on the number of active elements and nodes of the network. Consequently, the performance of these approaches depends on the considered network and there is no clear winner within our approaches that dominates the others in general.

As explained in [JT5] in more detail, we finally highlight that especially our characterization to decide FB w.r.t. (WBFA), e.g., the one in Theorem 6.5.5, have potential to include expert knowledge of the TSO to decide the feasibility of a booking. For example, if the TSO is aware of bottlenecks of the network, then the TSO may be able to decide the infeasibility of a given booking by only solving specific subproblems of the obtained characterizations containing this bottleneck.

6.6. Robust Diameter Sizing for Tree-Shaped Hydrogen Networks

In this section, we exemplarily outline how our results for deciding the feasibility of a booking FB can also contribute to other potential-based network problems with demand uncertainties. To this end, we consider the problem of computing a diameter selection for a given passive and tree-shaped hydrogen pipeline network, in which the diameter selection needs to be protected against future demand fluctuations. We note that the sketched methodology to obtain a robust diameter selection is developed in [JT10][2] and we also apply it in our application-driven article [JT6].

As described in [JT10], we can model a robust diameter selection with minimal costs for our potential-based flow model (PBF) and a passive tree-shaped network $G = (V, A)$ by the two-stage robust mixed-integer nonlinear problem

$$
\begin{aligned}
\min_x \quad & \sum_{a \in A} \sum_{d \in D_a} c_{a,d} x_{a,d} && && (6.15a)\\
\text{s.t.} \quad & \sum_{d \in D_a} x_{a,d} = 1, && a \in A, && (6.15b)\\
& x_{a,d} \in \{0,1\}, && a \in A, d \in D_a, && (6.15c)\\
& \text{s.t.} \quad \forall \ell \in N(b)\ \exists q, \pi \text{ with } (4.3), (\text{PBF b}), && && (6.15d)\\
& \qquad \pi_u - \pi_v = \psi_a\Big(\sum_{d \in D_a} d x_{a,d}, q_a\Big), && a = (u,v) \in A, && (6.15e)
\end{aligned}
$$

where D_a is the finite set of diameters that can be selected for arc $a \in A$ and $c_{a,d} \in \mathbb{R}$ denotes the costs for diameter $d \in D_a$ and arc $a \in A$. Further, $\psi_a(d, \cdot)$ is a potential function satisfying Definition 4.2.3 for every $a \in A$, which additionally depends on the chosen diameter $d \in D_a$. The given load flow $b \in L$, which is called capacity scenario instead of booking in the considered context, determines our uncertainty set $N(b)$ consisting of all balanced load flows within b as introduced in Definition 5.1.2. Thus, the uncertainty set generally contains infinitely many nominations representing the uncertain future supply and demand of hydrogen.

The objective function (6.15a) minimizes the aggregated costs for the selected diameters. The first-stage constraints (6.15b) and (6.15c) ensure that we choose exactly one diameter for each pipe. These "here-and-now" decisions are discrete since in practice usually only specific sizes of diameters are available. By Constraints (6.15e), we model the effect of the chosen diameter on the potential levels. For fixed flow, a larger diameter leads to a smaller potential drop in the pipe and choosing a smaller

[2] We would like to note that [JT10] is not part of this dissertation; see author's contribution.

diameter instead usually increases the potential drop, but decreases the costs. The second-stage constraints (6.15d) and (6.15e) ensure that the computed diameter selection is protected against demand fluctuations within $N(b)$, i.e., every balanced load flow in $N(b)$ can be transported through the network.

For a fixed diameter selection, i.e., a fixed assignment of x, the Constraints (6.15d) and (6.15e) are equivalent to the problem of deciding the feasibility of the booking b for the potential-based flow model (PBF). Consequently, we can equivalently replace our uncertainty set $N(b)$ by a finite set of "special" scenarios called finite feasible design set in [JT10]. This set can be obtained by computing for the finitely many possible diameter selections the corresponding maximum potential difference inducing nominations; which e.g., follows from Theorem 7 and 10 in [81]. More precisely, for every assignment of x and node pair, we solve Problem (6.1) and add the obtained nominations to our finite feasible design set. However, the obtained finite feasible design set can be extremely large in general. Fortunately, for the case of tree networks, our nominations with maximum potential differences solely depend on the tree structure of the network and are independent from the potential functions as explained in Section 6.3.1. Exploiting this, it is shown in [JT10] that under mild assumptions on the potential bounds a finite feasible design set consisting of $|V_+| \times |V_-|$ many nominations exists. Moreover, the two-stage robust nonlinear problem (6.15) can be reformulated as a finite-dimensional mixed-integer problem in tree-shaped networks; see [JT10].

We applied the sketched methodology of [JT10] to compute a robust diameter selection for different tree-shaped hydrogen networks in our application-driven article [JT6]. We note that in [JT6] we focus on comparing a linear and nonlinear model for pipe sizing w.r.t. the investment costs. The results of [JT6] show that the nonlinear model leads to smaller overall costs compared to the linear model. However, this saving is rather small taking into account the overall electrical reconversion costs. Thus, in [JT6] it is not recommended to include nonlinear models into energy system models, which are usually large-scale models and in addition to the selection of diameters also consider further aspects of designing a network. But it is suggested to apply the nonlinear model for pipe sizing as post-processing to verify the feasibility of the results. This is mainly based on the computational performance of the nonlinear model that is generally more challenging than the one of the linear model. However, if only the computation of a robust diameter selection is considered instead of optimizing a complete energy system, then the reformulated model of (6.15) can be solved well in practice; see [JT10]. In general, the author of this dissertation believes that it is beneficial to integrate such nonlinear models in large-scale energy system models in the long run since the obtained results are usually closer to reality than for the case of linear models. Furthermore, considering demand uncertainties within the network optimization process, e.g., using the sketched robust optimization approach, improves the reliability of the designed network.

Overall, the example of robust diameter sizing shows that the results of deciding the feasibility of a booking can also contribute to further network problems with demand uncertainties. Based on the results for FB, we now turn to the computation of maximal technical capacities in the next chapter, which can be seen as computing a maximal booking.

7. Gas Flows with Load Flow Uncertainties: Maximal Uncertainty Sets on Trees

In this chapter, we summarize our results of [JT7] and [JT8] for the problem of computing maximal technical capacities (CTC). As described in Section 5.1, this problem aims at computing a maximal uncertainty set of balanced load flows such that each of these flows can be transported through the network. We use the definitions and notations introduced in Section 5.1 and consider our gas transport models of Section 4.2. As described in [JT7], the decision variant of computing maximal technical capacities (5.3) in passive networks is formally given by

Computing Technical Capacities (CTC)

Input: A weakly connected Graph $G = (V, A)$ with entries V_+, exits V_-, inner nodes V_0, constraints $c_{\mathcal{E}}(x; \ell) = 0$ and $c_{\mathcal{I}}(x; \ell) \geq 0$, a weight vector $d \in \mathbb{Q}^V$, and threshold value $T \in \mathbb{Q}_{\geq 0}$.

Question: Do feasible technical capacities $q^{\mathrm{TC}} \in F_{\mathrm{C}}$ satisfying (5.3b) and (5.3c) with $d^T q^{\mathrm{TC}} \geq T$ exist, i.e.,
$\exists q^{\mathrm{TC}} \in C$ satisfying (5.3b) and (5.3c) with $d^T q^{\mathrm{TC}} \geq T$ such that
$\forall \ell \in N(q^{\mathrm{TC}}) = \left\{\ell \in L \,:\, \ell \leq q^{\mathrm{TC}}, \sum_{u \in V_+} \ell_u = \sum_{u \in V_-} \ell_u\right\}$
$\exists x \in \mathbb{R}^n$ satisfying $c_{\mathcal{E}}(x; \ell) = 0,\ c_{\mathcal{I}}(x; \ell) \geq 0$?

Constraints $c_{\mathcal{E}}(x; \ell) = 0$ and $c_{\mathcal{I}}(x; \ell) \geq 0$ denote one of our models for gas transport in passive networks; see Section 4.2. Since we study CTC also from the perspective of computational complexity, we assume in line with Chapter 6 that all constants within constraints $c_{\mathcal{E}}(x; \ell) = 0$ and $c_{\mathcal{I}}(x; \ell) \geq 0$ are rational and consider a classical Turing machine as our computational model in the corresponding section; see [53]

This chapter is outlined as follows. In Section 7.1, we discuss the hardness results developed in [JT7], which prove that CTC is NP-hard for capacitated linear flows (CLF) as well as for linear and nonlinear potential-based flows (WBF). This holds even for tree-shaped networks, which emphasizes the difficulty of CTC. In Section 7.2, we provide a finite-dimensional convex mixed-integer model for computing maximal technical capacities (5.3) in tree-shaped passive networks developed in [JT8]. In addition, we present combinatorial constraints of [JT8] that significantly speed up the solution process. Finally, we briefly discuss how this model is successfully applied in [JT8] to solve the multilevel model of the European entry-exit gas market of [64] for a tree-shaped passive network of real-world size and nonlinear flow model (WBF).

All of the following results originate from [JT7] and [JT8]. Throughout this chapter, we follow the corresponding description of these results within [JT7] and [JT8], to which we refer for a complete explanation including all proofs.

7.1. NP-Hardness

In [JT7], it is proven that computing technical capacities (CTC) is NP-hard for capacitated linear flows (CLF) as well as for linear and nonlinear potential-based flows (WBF). This holds even for tree-shaped networks. In the following, we roughly sketch the main idea of the hardness proof for the case of capacitated linear flows (CLF). We can reduce this case to the one of linear and nonlinear potential-based flows, see [JT7], since our hardness result is proven for trees and, thus, there is no cyclic flow in the network. Throughout this section, we denote technical capacities as feasible if they satisfy Definition 5.1.6 as well as Constraints (5.3b) and (5.3c).

In Section 3.1 of [JT7], it is proven that CTC is in NP for capacitated linear flows (CLF) in tree-shaped networks. To prove NP-hardness of CTC for (CLF), we reduce the Subset Sum problem to CTC.

Subset Sum (SSP).

Input:	$M \in \mathbb{N}$, $S_1, \dots, S_n \in \mathbb{N}$ with $S_i \leq M$ for $i \in \{1, \dots, n\}$, $n \geq 2$, and $\sum_{i=1}^{n} S_i \geq M$.
Question:	Does $I \subseteq \{1, \dots, n\}$ with $\sum_{i \in I} S_i = M$ exist?

We note that this variant slightly differs from the one in [53]. However, it is still NP-hard; see [JT7]. We only sketch the main idea of the hardness proof in the following since this proof is very technical. Our description is based on the one in [JT7], to which we refer for a detailed explanation including all proofs.

For a given SSP instance, we consider the graph $G(\mathsf{SSP}) = (V, A)$ for computing maximal technical capacities w.r.t. (CLF), which is illustrated by Figure 7.1 including the corresponding arc flow bounds. A complete description of the corresponding CTC instance including the weight vector $d \in \mathbb{R}^V$ and the threshold value $T(\mathsf{SSP})$ is given in [JT7]. Moreover, we denote technical capacities that correspond to an optimal solution of the optimization problem (5.3) that computes maximal technical capacities as optimal technical capacities in the following. Using several auxiliary results, it is proven in [JT7] that the objective value of optimal technical capacities in $G(\mathsf{SSP})$ is at least the threshold value $T(\mathsf{SSP})$ if and only if Subset Sum is feasible.

Lemma 7.1.1 (Lemma 3.18 in [JT7])**.** *The SSP problem is solvable if and only if the optimal technical capacities $q^{\mathrm{TC}} \in C$ w.r.t. capacitated linear flows (CLF) in $G(\mathsf{SSP})$ satisfy*

$$d^T q^{\mathrm{TC}} \geq T(\mathsf{SSP}).$$

We now sketch the main idea for proving this result. From combining Lemmas 3.11, 3.13, and 3.17 of [JT7], it follows that optimal technical capacities q^{TC} in $G(\mathsf{SSP})$ with $d^T q^{\mathrm{TC}} \geq T(\mathsf{SSP})$ satisfy the following properties

$$\sum_{i=1}^{n} q^{\mathrm{TC}}_{h_i} = M, \quad 0 \leq q^{\mathrm{TC}}_{h_i} \leq S_i,\ i \in \{1, \dots, n\}. \tag{7.1}$$

Thus, we are already close to solving the SSP instance under consideration since we now only have to ensure that it is beneficial to chose $q^{\mathrm{TC}}_{h_i} \in \{0, S_i\}$ for all $i \in \{1, \dots, n\}$

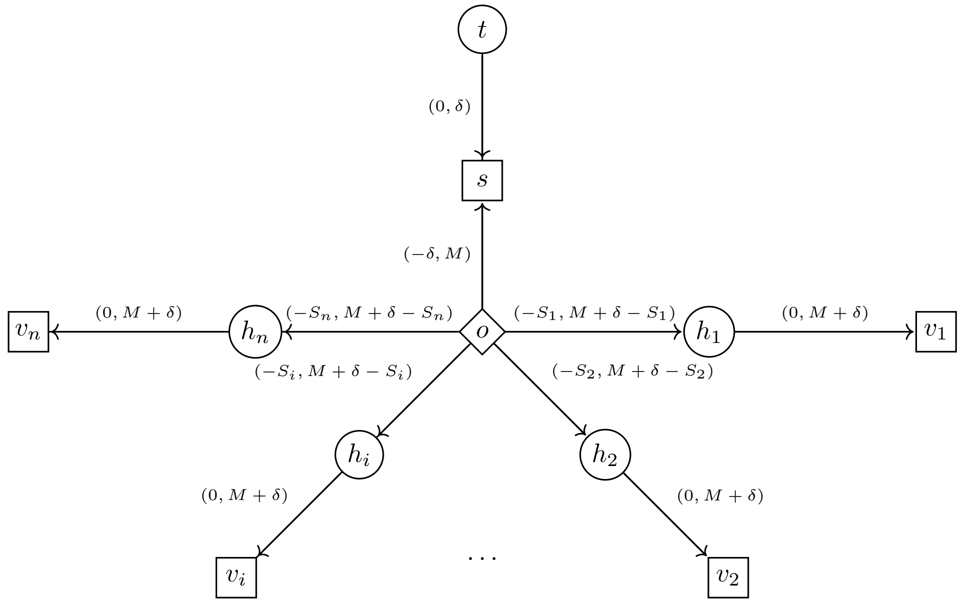

Figure 7.1.: The graph $G(\mathsf{SSP})$. Entry nodes are indicated by circles, exits by boxes, and inner nodes by diamonds. The corresponding lower and upper arc flow bounds are given by (q_a^-, q_a^+) using the abbreviation $\delta = (n+1)^{-1}$. Here, $n \in \mathbb{N}$ denotes the number of elements of the considered SSP instance; adapted version of [JT7, Figure 1; licensed under CC BY 4.0].

if this is feasible. As shown in [JT7], this is guaranteed by the construction of the $G(\mathsf{SSP})$ instance since for optimal technical capacities q^{TC} with $d^T q^{\mathrm{TC}} \geq T(\mathsf{SSP})$ the objective value of the ith branch of $G(\mathsf{SSP})$ is maximal if $q_{h_i}^{\mathrm{TC}} \in \{0, S_i\}$ for $i \in \{1, \dots, n\}$ holds, i.e.,

$$d_{h_i} q_{h_i}^{\mathrm{TC}} + d_{v_i} q_{v_i}^{\mathrm{TC}} = \begin{cases} M + \delta - S_i, & q_{h_i}^{\mathrm{TC}} \in \{0, S_i\}, \\ -q_{h_i}^{\mathrm{TC}} + M + \delta - S_i, & q_{h_i}^{\mathrm{TC}} \in (0, S_i). \end{cases} \tag{7.2}$$

Equation (7.2) follows from Conditions (7.1) and applying a case distinction regarding Lemmas 3.14 and 3.15 of [JT7] as it is done in the proof of Lemma 3.16 in [JT7].

If the considered SSP instance is feasible, then we can satisfy Conditions (7.1) such that $q_{h_i}^{\mathrm{TC}} \in \{0, S_i\}$ holds for all $i \in \{1, \dots, n\}$. Consequently, for all $i \in \{1, \dots, n\}$ the objective value of the ith branch evaluates to $M + \delta - S_i$, which is maximal due to Equation (7.2). This is one of the main reasons why the corresponding optimal solution exceeds the considered threshold value $T(\mathsf{SSP})$ if the SSP instance is feasible; see Lemma 3.9 in [JT7].

However, if the SSP instance is infeasible, then we can satisfy Conditions (7.1) only such that $q_{h_i}^{\mathrm{TC}} \in (0, S_i)$ for at least one index $i \in \{1, \dots, n\}$ holds. Thus, the corresponding objective value of this branch is $-q_{h_i}^{\mathrm{TC}} + M + \delta - S_i$ due to (7.2), which is lower compared to the case if SSP is feasible. This is one of the main reasons why the optimal value does not exceed the threshold value $T(\mathsf{SSP})$ if the SSP instance is infeasible, see Lemma 3.16 and 3.17 in [JT7].

Theorem 7.1.2 (Theorem 3.19, 4.9, and 4.10 in [JT7]). *Computing maximal technical capacities (CTC) w.r.t. capacitated linear flows (CLF), linear potential-based flows, and nonlinear-potential-based flows (WBF) is NP-complete on passive trees. On general graphs, it is at least NP-hard.*

In Theorem 4.9 and 4.10 of [JT7], it is proven that we can transfer the hardness result for CTC with capacitated linear flows to the case of linear and nonlinear potential-based flows by replacing the arc flow bounds by specific potential bounds.

We finally note that computing maximal technical capacities (CTC) is NP-hard even on trees whereas deciding their feasibility can be done in polynomial time for tree-shaped networks, see Section 6.3.1, and for linear potential-based flows in general graphs; see [81]. In the next section, we now move on to the computation of technical capacities within a multilevel model of the European entry-exit gas market [64].

7.2. Computing Maximal Technical Capacities on Trees

In the previous section, we solely focused on the computation of maximal technical capacities modeled by (5.3). This model results from a multilevel model of the European entry-exit gas market system [64] to directly address one of its core difficulty, namely the computation of feasible technical capacities; see Section 5.1 for more details. In [JT8], we now consider the entire multilevel model of the European entry-exit gas market of [64], which can be reformulated as a bilevel problem; see [64]. As core difficulty this model contains the computation of feasible technical capacities modeled by (5.3d) with the goal of maximizing the social welfare. We now discuss a reformulation for the nonlinear adjustable robust constraints (5.3d) modeling feasible technical capacities, which is developed in [JT8]. We focus on our nonlinear Weymouth based gas transport model (WBF) and assume that the underlying network is a tree. Our model consists of finitely many convex constraints with additional integer variables, which is quite surprising since the considered model of gas transport (WBF) itself is nonconvex.

We note that the presented modeling approach is developed in [JT8] and we follow its description within [JT8] throughout this section. To do so, we denote technical capacities as optimal if they correspond to an optimal solution of the bilevel reformulation of the considered market model; see [64]. Moreover, we use the notation of Section 6.3.1 in the following.

Since technical capacities can be seen as a booking, it follows from Section 6.3.1 and [81] that technical capacities $q^{\mathrm{TC}} \in \mathbb{R}^V_{\geq 0}$ are feasible if and only if for each pair of nodes $(w_1, w_2) \in V^2$ they satisfy

$$\sum_{a \in A^{\rightarrow}(w_1,w_2)} \Lambda_a \xi_a^+ (q^{\mathrm{TC}})^2 + \sum_{a \in A^{\leftarrow}(w_1,w_2)} \Lambda_a \xi_a^- (q^{\mathrm{TC}})^2 \leq \pi_{w_1}^+ - \pi_{w_2}^-,$$

where the lower $\xi_a^-(q^{\mathrm{TC}})$ and upper $\xi_a^+(q^{\mathrm{TC}})$ arc flow bounds for arc $a \in A$ are given by (6.3). Further, $A^{\rightarrow}(w_1, w_2)$ represents the arcs of the unique flow-path $P(w_1, w_2)$ that are directed from w_1 to w_2 and $A^{\leftarrow}(w_1, w_2)$ contains the remaining arcs of $P(w_1, w_2)$; see Section 6.3.1.

The main idea of our model consists of explicitly representing the lower $\xi_a^-(q^{\mathrm{TC}})$ and upper $\xi_a^+(q^{\mathrm{TC}})$ arc flow bounds using additional integer variables and the following big-Ms

$$M^+ \geq \sum_{u \in V_+} q_u^{\mathrm{TC}}, \quad M^- \geq \sum_{u \in V_-} q_u^{\mathrm{TC}}. \tag{7.3}$$

By Lemma 3.5 in [JT8], it is shown how to a priori compute finite $M^+ \in \mathbb{R}$ and $M^- \in \mathbb{R}$ so that (7.3) holds for at least one bilevel optimal solution, respectively the corresponding optimal technical capacities. We now present our convex mixed-integer model of [JT8], which contains bilinear terms that can be reformulated by using the big-Ms M^+ and M^- as described in Lemma 4.9 in [JT8].

$$\begin{aligned}
&\bar{h}^+_{(u,v)} = \sum_{w \in V_+ \cap V_u^{(u,v)}} q_w^{\mathrm{TC}}, && (u,v) \in A, && \text{(7.4a)}\\
&\bar{h}^-_{(u,v)} = \sum_{w \in V_- \cap V_v^{(u,v)}} q_w^{\mathrm{TC}}, && (u,v) \in A, && \text{(7.4b)}\\
&\bar{h}^+_{(u,v)} - \bar{h}^-_{(u,v)} \leq M^+ \bar{x}_{(u,v)}, && (u,v) \in A, && \text{(7.4c)}\\
&\bar{q}_{(u,v)} = \bar{h}^+_{(u,v)}(1 - \bar{x}_{(u,v)}) + \bar{h}^-_{(u,v)} \bar{x}_{(u,v)}, && (u,v) \in A, && \text{(7.4d)}\\
&\underline{h}^+_{(u,v)} = \sum_{w \in V_+ \cap V_v^{(u,v)}} q_w^{\mathrm{TC}}, && (u,v) \in A, && \text{(7.4e)}\\
&\underline{h}^-_{(u,v)} = \sum_{w \in V_- \cap V_u^{(u,v)}} q_w^{\mathrm{TC}}, && (u,v) \in A, && \text{(7.4f)}\\
&\underline{h}^+_{(u,v)} - \underline{h}^-_{(u,v)} \leq M^+ \underline{x}_{(u,v)}, && (u,v) \in A, && \text{(7.4g)}\\
&\underline{q}_{(u,v)} = \underline{h}^+_{(u,v)}(1 - \underline{x}_{(u,v)}) + \underline{h}^-_{(u,v)} \underline{x}_{(u,v)}, && (u,v) \in A, && \text{(7.4h)}\\
&\bar{q}_a^2 \leq \bar{f}_a, && a \in A, && \text{(7.4i)}\\
&\underline{q}_a^2 \leq \underline{f}_a, && a \in A, && \text{(7.4j)}\\
&\sum_{a \in A^{\rightarrow}(u,v)} \Lambda_a \bar{f}_a + \sum_{a \in A^{\leftarrow}(u,v)} \Lambda_a \underline{f}_a \leq \pi_u^+ - \pi_v^-, && (u,v) \in V^2, && \text{(7.4k)}\\
&\underline{x}_a, \bar{x}_a \in \{0,1\}, \ q_v^{\mathrm{TC}} \geq 0, && a \in A, \ v \in V, && \text{(7.4l)}
\end{aligned}$$

Here, $V_v^{(u,v)}$ denotes the set of nodes of the subtree that contains v after removing arc $(u,v) \in A$; see Section 6.3.1. As described in [JT8], Constraints (7.4a)–(7.4d) ensure that $\bar{q}_a$ is at least as large as the upper arc flow bound $\xi_a^+(q^{\mathrm{TC}})$, i.e., $\bar{q}_a \geq \xi_a^+(q^{\mathrm{TC}})$. In analogy, Constraints (7.4e)–(7.4h) ensure $\underline{q}_a \geq |\xi_a^-(q^{\mathrm{TC}})|$. Moreover, Constraints (7.4i) and (7.4j) are a modeling choice that enables us to linearly model the flow in Constraints (7.4k). This reduces the number of convex constraints. Further, Constraints (7.4k) ensure that for every pair of nodes the corresponding maximum potential difference within the considered technical capacities is bounded by the relevant potential bounds. This guarantees the feasibility of the considered technical capacities.

In [JT8], it is shown that every feasible point of System (7.4) provides feasible technical capacities that satisfy Constraints (5.3d); see Lemma 4.6 in [JT8]. Moreover, it is shown that there is at least one optimal solution of the bilevel reformulation of the considered market model such that the corresponding technical capacities can be extended to a feasible point of our model; see Lemmas 3.5 and 4.5 in [JT8]. Consequently, we can replace the nonlinear adjustable robust constraints (5.3d) by our finite-dimensional convex mixed-integer constraints (7.4) in the considered multilevel model of the European entry-exit gas market system. In doing so, we can equivalently reformulate the bilinear terms in Constraints (7.4) using the big-M values M^+ and M^-, which leads to a model consisting of finitely many convex constraints with additional binary variables; see Section 4 of [JT8].

Applying our presented model to the multilevel model of the European entry-exit gas market [64] enables us to recast this multilevel model to a finite-dimensional mixed-integer nonlinear optimization problem as described in [JT8]. This problem can now be solved by optimization software such as Gurobi [66]; see Section 7.3.

As described in [JT8], our Model (7.4) can also be applied to our general potential-based flow model (PBF) by replacing (7.4k) with

$$\sum_{a \in A^{\rightarrow}(u,v)} \psi_a(\bar{q}_a) + \sum_{a \in A^{\leftarrow}(u,v)} \psi_a(\underline{q}_a) \leq \pi_u^+ - \pi_v^-, \quad (u,v) \in V^2,$$

where ψ_a is a potential loss function for $a \in A$ that satisfies Definition 4.2.3. For general potential-based flows this constraint is not necessarily convex anymore. We note that we can neglect Constraints (7.4i) and (7.4j) in the general case since these constraints are specific for the considered model (WBF) to reduce the number of convex constraints.

To conclude this section, we present additional combinatorial constraints for Model (7.4) developed in [JT8]. These constraints significantly speed up the solution process of the considered market model; see Section 7.3 and [JT8]. In the following, $\lceil x \rceil$ denotes rounding up the value x.

Lemma 7.2.1 (Lemma 5.2 in [JT8]). *Let $G = (V, A)$ be a tree and $\left(\bar{f}, \underline{f}, \bar{q}, \underline{q}, \underline{h}^-, \bar{h}^-, \underline{h}^+, \bar{h}^+, \underline{x}, \bar{x}, q^{\mathrm{TC}}\right)$ [1] a feasible point of (7.4) that for arc $a = (u, v) \in A$ satisfies*

$$\bar{x}_{(u,v)} = \max\left\{0, \left\lceil \frac{1}{M^+}(\bar{h}^+_{(u,v)} - \bar{h}^-_{(u,v)}) \right\rceil \right\}, \tag{7.5a}$$

$$\underline{x}_{(u,v)} = \max\left\{0, \left\lceil \frac{1}{M^+}(\underline{h}^+_{(u,v)} - \underline{h}^-_{(u,v)}) \right\rceil \right\}. \tag{7.5b}$$

Then, the inequalities

$$\bar{x}_{(u,v)} \leq \bar{x}_{(v,l)}, \quad (v,l) \in \delta^{\mathrm{out}}(v), \tag{7.6a}$$

$$\underline{x}_{(v,l)} \leq \underline{x}_{(u,v)}, \quad (v,l) \in \delta^{\mathrm{out}}(v), \tag{7.6b}$$

$$\bar{x}_{(u,v)} \leq \underline{x}_{(l,v)}, \quad (l,v) \in \delta^{\mathrm{in}}(v), \tag{7.6c}$$

are satisfied for $a = (u, v) \in A$.

[1] We note that all entries of the vector have to be transposed, but to simplify notation we omit this and maintain this convention throughout this section.

For every feasible point of System (7.4), there exists a feasible point of System (7.4) with the same exact feasible technical capacities that satisfies Equations (7.5) for every arc; see Lemma 5.1 in [JT8]. Consequently, we can add the derived additional combinatorial constraints (7.6) to our Model (7.4) without cutting off feasible technical capacities.

Following the description within [JT8], we now sketch the main intuition of our combinatorial constraints on the example of Constraints (7.6a), which is based on the tree-shaped network structure. To do so, we consider a feasible point $\left(\bar{f}, \underline{f}, \bar{q}, \underline{q}, \underline{h}^-, \bar{h}^-, \underline{h}^+, \bar{h}^+, \underline{x}, \bar{x}, q^{\mathrm{TC}}\right)$ of Model (7.4) satisfying Equations (7.5) and an arc $(u, v) \in A$. If $\bar{x}_{(u,v)} = 1$ holds, then from Constraints (7.4d) and Conditions (7.5) it follows

$$\bar{q}_{(u,v)} = \min \left\{ \sum_{w \in V_+ \cap V_u^{(u,v)}} q_w^{\mathrm{TC}}, \sum_{w \in V_- \cap V_v^{(u,v)}} q_w^{\mathrm{TC}} \right\} = \sum_{w \in V_- \cap V_v^{(u,v)}} q_w^{\mathrm{TC}} = \bar{h}^-_{(u,v)}.$$

For an outgoing arc (v, l), we now consider variable $\bar{q}_{(v,l)}$. Thus, there are possibly more entries that can supply flow via (v, l) due to $V_u^{(u,v)} \subset V_v^{(v,l)}$. Furthermore, there are possibly less exits that can receive flow via arc (v, l) due to $V_l^{(v,l)} \subset V_v^{(u,v)}$. Consequently, the value of $\bar{q}_{(v,l)}$ corresponds to the aggregated technical capacities of the exits, i.e., $\bar{q}_{(v,l)} = \bar{h}^-_{(v,l)}$ and $\bar{x}_{(v,l)} = 1$ hold, due to Constraints (7.4c) and (7.4d) as well as Conditions (7.5). Moreover, we now explicitly enforce $\bar{x}_{(v,l)} = 1$ by Constraints (7.6a).

In the next section, we demonstrate how Model (7.4) and the additional combinatorial constraints (7.6) are successfully applied to the considered multilevel model of the European entry-exit gas system [64].

7.3. Solving a Multilevel Model of the European Entry-Exit Gas Market System on a Real-World Sized Tree Network

We now briefly discuss our computational results of [JT8], in which we solve a multilevel model of the European entry-exit gas market system, developed in [64], for a real-world sized tree network and nonlinear gas flows (WBF). For a brief introduction to the European entry-exit gas market system and the considered multilevel model, we refer to Section 5.1, [JT8], and [64]. So far in the literature, the considered multilevel model is solved for simplified linear potential-based flows and stylized small (but cyclic) passive networks; see [26]. However, we now focus on our nonlinear potential-based flow model (WBF) in real-world sized tree-shaped networks consisting only of pipes.

As described in [JT8], the considered multilevel model can be reformulated as a single level mixed-integer nonlinear optimization problem. However, the obtained reformulation cannot be solved computationally in general since it includes the

Table 7.1.: Number of solved instances (out of 110 instances) and statistics for the runtimes (always taken only for all instances solved to optimality); adapted version of [JT8, Table 2; licensed under CC BY 4.0].

	comb-cons	w/o comb-cons
#solved	107	87
	Time (s)	Time (s)
Minimum	251.65	2069.42
1st Quartile	670.65	9790.43
Median	1070.32	17 685.29
3rd Quartile	2127.64	41 813.73
Maximum	32 833.46	83 639.78

nonlinear adjustable robust constraints (5.3d) modeling feasible technical capacities. Applying our finite-dimensional model (7.4) for these Constraints (5.3d) leads to a finite-dimensional single level mixed-integer nonlinear model that can be solved with optimization software such as Gurobi [66]. In [JT8], we solve this reformulation for a passive version of the Greek gas network, which is a tree and is represented by the instance GasLib 134 of [102]. For a complete description of our economic and computational setup including the generation of our 110 economic instances, we refer to Section 6 in [JT8].

In this summary, we highlight the computational benefit of including our additional combinatorial constraints of Section 7.2. To do so, we follow the description of our results within [JT8]. Our single-level reformulation consists of 3599 variables, of which 698 are binary variables, and of 22085 constraints, of which 267 are quadratic constraints. We further have 266 combinatorial constraints given by Inequalities (7.6). The runtimes for the considered 110 instances w.r.t. GasLib-134 are summarized in Table 7.1. We can solve 107 out of 110 instances to global optimality within the time limit of 24 h and 90 of these instances are solved within 1 h. Our combinatorial constraints (7.6) play a key role in obtaining these short runtimes, which is pointed out by the fact that the minimum runtime excluding them is close to the third quartile of the runtimes including the combinatorial constraints. Further analysis in [JT8] show that the observed computational speed up by including our combinatorial constraints can be explained by the observation that these constraints significantly reduce the number of explored nodes within the branch-and-bound solution process.

For an exemplary analysis of the sensitivity of our approach regarding changes in the economic input data, e.g., changes of the demand, we refer to [JT8].

Overall, this is the first time that the considered multilevel entry-exit gas market model has been solved for a real-world sized passive network and a nonlinear gas flow model.

8. Evaluation and Outlook

We now briefly evaluate our obtained results w.r.t. the described challenges in Section 1.1. Additionally, we sketch possible steps for future research.

In Chapter 3, we studied the radius of robust feasibility (RRF) for mixed-integer linear problems (MIPs) to determine the maximal size of a given uncertainty such that robust feasibility is still guaranteed. We introduced and analyzed the RRF for MIPs in the common setting of the literature. Afterward, we extended the framework of the RRF to include "safe" variables and constraints, i.e., variables and constraints that are not affected by uncertainties. We further developed first methods for computing the RRF of LPs and MIPs including safe variables and constraints and successfully applied these methods to instances of the MIPLIB 2017 library. Thus, we addressed the challenges that the RRF is only studied for continuous optimization problems without safe variables or constraints in the literature. Consequently, our results allow to apply the RRF to a broader variety of applications, which usually contain safe variables and constraints. Additionally, we suggested a strategy that allows to "control" the so-called price of robustness by adjusting the size of a given uncertainty set using our results for the RRF; see Section 3.5.

Despite our significant progress w.r.t. the RRF, many related research possibilities remain. As a first step, it seems promising for different applications to evaluate the benefit of choosing the size of the uncertainty set in the optimization process to control the price of robustness as outlined in Section 3.5. This is directly possible using the results of this cumulative dissertation. In addition, further methods for computing the RRF including safe variables and constraints are desirable. To provide a more "flexible" choice of the size of the uncertainty set, a different radius can be assigned to every uncertain constraint. This requires the development of solution methods that, for example, maximize the sum of different radii. From a more macroscopic perspective, the results of the RRF may contribute to the question: "Can we trade a small amount of robustness, i.e., a small reduction of the uncertainty set, for a large decrease in the price of robustness?", which is an interesting research question in the long run.

We studied the two-stage robust problems of deciding the feasibility of a booking as well as of computing maximal technical capacities within the European entry-exit gas market system in Chapters 5–7. For both problems, we focused on nonlinear potential-based models for gas transport. Aside from minor technical subtleties, the considered problems correspond to deciding the feasibility as well as solving a specific two-stage nonlinear robust optimization problem. This robust problem aims at computing a maximal uncertainty set of balanced load flows such that each of these load flows can be transported through the network. We studied this specific two-stage robust problem algorithmically in Chapters 6 and 7. We analyzed structural properties such as (non-)convexity and star-shapedness of the set of feasible bookings and of the set of feasible balanced load flows for different models of gas transport. In [81], it is shown that the feasibility of a booking can be decided in polynomial time in pipe-only trees, which can also be derived by our results using a slightly different approach. For single-cycle networks consisting only of pipes, we developed a method that decides the feasibility of a booking in polynomial time. However, this task is proven to be coNP-hard in general pipe-only networks. We additionally characterized feasible bookings in networks with compressors and control valves. Based on the results for bookings, we provided first steps for computing maximal technical capacities in tree-shaped passive networks. The results allow us to solve a multilevel model of the European entry-exit gas market system from the literature [64] for a tree-shaped passive network of real-world size and a nonlinear gas flow model. We remark that our results can also contribute to other potential-based network problems, e.g., for computing a robust diameter selections for tree-shaped hydrogen networks with demand uncertainties. Overall, we addressed the challenges posed by the nonlinear gas transport by exploiting the underlying network structure as well as structural properties of the considered potential-based gas flow models. This also enables us to provide first results for the case of active elements under the assumption that the active elements do not lie on cycles of the network. We note that these active elements such as compressors and control valves lead to challenging adjustable integer variables. Additionally, we provided results for computing maximal technical capacities, which form a challenging decision-dependent uncertainty set.

There are many possible options for future research. To start with, the development of methods for computing maximal technical capacities of general networks is desirable. Due to the difficulty of this problem, it can be a smart choice to consider approximation algorithms for computing technical capacities. Further, the development of approaches for deciding the feasibility of a booking in active networks without any assumption on the location of the active elements is an interesting problem. Moreover, we believe that taking into account the corresponding market system in the optimization process of network planning and expansion poses a rewarding challenge for future research. It possibly allows to resolve bottlenecks of the network resulting from the considered market system. For example, on the basis of our results, the multilevel model of the European entry-exit gas market system [64] can be further developed to include the option of expanding the capacity of certain pipelines in order to possibly resolve bottlenecks resulting from the entry-exit system.

In the long run, it seems promising to expand our research on potential-based flows for general network problems such as network expansion since the use of general potential-based flows allows to apply the results to a variety of different applications, e.g., hydrogen, water, or lossless DC power networks. Further, specific properties of potential-based flows, e.g., uniqueness of flows in passive networks, together with the underlying network structure can be used to derive solution approaches as we have demonstrated by our results. The author of this dissertation believes that one of the most promising starting points for future research consists of studying the extension of our results to uncertain potential-based network problems with general demand uncertainties, i.e., we replace our application-driven uncertainty set by a general convex and compact uncertainty set of balanced load flows.

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Part B

Reprint of Published Articles and Preprints

Article 1

Radius of Robust Feasibility for Mixed-Integer Problems

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Radius of Robust Feasibility for Mixed-Integer Problems

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Abstract. For a mixed-integer linear problem (MIP) with uncertain constraints, the radius of robust feasibility (RRF) determines a value for the maximal "size" of the uncertainty set such that robust feasibility of the MIP can be guaranteed. The approaches for the RRF in the literature are restricted to continuous optimization problems. We first analyze relations between the RRF of a MIP and its continuous linear (LP) relaxation. In particular, we derive conditions under which a MIP and its LP relaxation have the same RRF. Afterward, we extend the notion of the RRF such that it can be applied to a large variety of optimization problems and uncertainty sets. In contrast to the setting commonly used in the literature, we consider for every constraint a potentially different uncertainty set that is not necessarily full-dimensional. Thus, we generalize the RRF to MIPs as well as to include "safe" variables and constraints, i.e., where uncertainties do not affect certain variables or constraints. In the extended setting, we again analyze relations between the RRF for a MIP and its LP relaxation. Afterward, we present methods for computing the RRF of LPs as well as of MIPs with safe variables and constraints. Finally, we show that the new methodologies can be successfully applied to the instances in the MIPLIB 2017 for computing the RRF.

1. Introduction

Robust optimization is a well-established method for protecting an optimization problem from data uncertainties that are usually defined via so-called uncertainty sets. Such data uncertainties may arise as a result of estimation and prediction errors as well as from a lack of (future) information. Robust optimization plays an important role in many applications such as finance, energy, supply chain, health care, etc., see [25] and the literature therein. For detailed overviews of the research area of robust optimization, we refer to [3, 5, 7, 10, 25]. One of the main goals consists in finding robust feasible solutions, i.e., solutions which are feasible for all realizations of a given uncertainty set. A solution is robust optimal if it is robust feasible and attains the best possible objective value. The corresponding robust optimization problem, also called robust counterpart, is, in general, semi-infinite. Nevertheless, for several important classes of optimization problems and uncertainty sets, it is possible to reformulate the robust counterpart as an algorithmically tractable finite optimization problem. This is in particular true for mixed-integer linear optimization and convex uncertainty sets, see for example [4] for a comprehensive treatment.

Intensive research has been conducted in developing algorithmically tractable robust counterparts. However, in applications it also important to construct appropiate uncertainty sets. Some proposals for constructing "good" uncertainty sets are given in [6, 8, 25]. High-volume uncertainty sets may lead to overly conservative solutions that are overly protected and furthermore lead to bad objective function

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values, when compared to the nominal solution. The overall goal of constructing "good" uncertainty sets consists in prohibiting too conservative, intractable, or even infeasible robust optimization problems due to the choice of the uncertainty set. In order to achieve these goals, it is useful to know the maximal "size" of a given uncertainty set such that a robust feasible solution still exists. In this paper, we study one notion of "size": the radius of robust feasibility (RRF). It is motivated by the notion of the consistency radius used in the linear semi-infinite programming, see [11–13].

In this work, we investigate the problem of determining the RRF for a mixed-integer linear optimization problem (MIP), both from a theoretical as well as from a practical point of view. To evaluate our methods on a set of realistic MIPs from different applications, we apply them to compute the RRF for the benchmark instances of the MIPLIB 2017 library.

In general, the RRF is defined as the supremum over all scaled sizes of a given uncertainty set such that robust feasibility is guaranteed. Consequently, it is possible that the supremum is not attained, i.e., the RRF is not attained. In this case, the uncertain problem is not feasible for the uncertainty set scaled by the RRF, but it is feasible for every smaller scaling, see [23]. The RRF has been researched only for continuous problems. For linear problems (LPs), theoretical and numerical tractable models for the RRF w.r.t. different compact and convex uncertainty sets are provided in [19, 23, 24]. The RRF is introduced in robust convex optimization in [22]. The authors further provide an upper bound of the RRF for convex problems with convex polynomial constraints and establish a method for computing the RRF of convex problems with SOS-convex polynomial constraints. In [18, 29], exact analytical formulas for the RRF of convex problems with general convex and compact uncertainty sets are established. We also note that in the recent paper [18] lower and upper bounds for the RRF of convex problems with different full-dimensional uncertainty sets for every constraint are given. We note that the RRF has connections to recent developments in the fields of stability and sensitivity analysis of robust optimization problems, see e.g., [16, 20], because it computes the solution that is most insensitive w.r.t. feasibility and changes, in form of scaling, of the uncertainty set.

We generalize the above-mentioned approaches in three directions: We allow that the uncertainty sets are different and not necessarily full-dimensional for every constraints. We do not require zero to be in the interior of the uncertainty set and finally, we allow integer variables in the optimization problem. This enables us to consider a wider variety of applications for the RRF. For instance, we can include "safe" constraints and variables, i.e., constraints and variables that are not affected by uncertainty. For example, if all coefficients of a constraint are deterministic, this constraint is safe. If all coefficients of some variable are deterministic in the constraint system, this variable is safe. The drawback of this generalization is, that we lose some of the nice theoretical properties of the RRF, e.g., finiteness, see [23]. Furthermore, the generalizations require the developement of new algorithmic techniques to compute the RRF.

The RRF has been studied for specific applications. For instance, in [14] the authors try to find the "most robust" facilities w.r.t. demand uncertainties for the Weber problem of facility location design. One can show that their problem is equivalent to computing the RRF. However, for this equivalence to hold, one cannot use the standard definition of the RRF, but one needs to extend it to include safe constraints and variables as in Section 3. The core idea in [14] is to remove the objective of the original problem and reintroduce it into the problem as a budget constraint for a fixed budget (e.g. the original optimal value). Then one can compute the RRF, with the budget constraint considered safe, to obtain a solution that can be seen as a "most robust" solution. The budget specifies how much a decision maker is willing to pay to obtain a robust solution. With the help of varying the budget, one can support decision makers by showing them the trade-off between robustness and worse objective values. With our work, the same idea can now be applied to general MIPs. The authors of [15] also use the concept of the RRF in facility location design. They consider a bi-objective problem that consists of maximizing robustness via the RRF and minimizing the estimated total cost. For LPs another example is the flexibility index problem, e.g., the RRF of an LP with a box uncertainty set, see [33].

A more complex variant of the RRF plays an important role in the context of design and control of gas networks. In the European Entry-Exit market system, the transmission system operator is obliged to allocate so called technical capacities in the network while guaranteeing the feasibility of the gas transport for any injection and withdrawal within these capacities, see [28] for a more detailed explanation. The computation of technical capacities leads to a two-stage nonlinear robust optimization problem that has not been solved in general so far. The latter problem can be solved by applying a complex variant of the extended RRF including "safe" constraints and variables and different radii for different constraints. Thus, this work is a first step towards computing technical capacities in gas network operations.

The key contributions of our paper are as follows:

(i) We first introduce the RRF for MIPs in Section 2. We then analyze in detail the relations between the RRF of a MIP and its LP relaxation in the common setting of the literature, i.e., where the uncertainty set is full-dimensional. We prove the main result that if the RRF of the LP relaxation is not attained, then this RRF equals the RRF of the corresponding MIP. The latter result enables us to compute the RRF of a MIP using known techniques for the RRF of LPs under certain conditions.

(ii) We extend the concept of the RRF to include "safe" variables and constraints in Section 3 in order to make the RRF applicable to a broader spectrum of problems and applications. We then again analyze relations between the RRF of a MIP and its LP relaxation. Further, we prove a necessary optimality condition for the RRF which is also sufficient under additional assumptions.

(iii) We provide first algorithms for computing the RRF including "safe" variables and constraints in Section 4. Finally, we present a computational study of the RRF w.r.t. the MIPLIB 2017 library, see [30]. We compare the performance of the proposed methods and the computed RRF. We also consider the *price of robustness* which measures the difference between the optimal objective value of the nominal problem and the corresponding value of the robust problem and discuss the obtained results.

2. Relations between the RRF of a MIP and of its LP Relaxation

In this section, we first introduce the radius of robust feasibility for a MIP and then relate it to that of its LP relaxation. In the following, let us consider a feasible MIP with coefficients $\bar{a}^j \in \mathbb{R}^n$ and $\bar{b}^j \in \mathbb{R}, j \in J$, of the constraints and finite index set $J \subset \mathbb{N}$ that is composed of

$$\min_{x \in \mathbb{Z}^k \times \mathbb{R}^{n-k}} \{c^T x \colon (\bar{a}^j)^T x \leq \bar{b}^j, j \in J\}. \tag{P}$$

For fixed $\alpha \geq 0$, let the robust counterpart for the uncertain MIP (P) with uncertainty set $\alpha\mathcal{U} \subseteq \mathbb{R}^{n+1}$ be given by

$$\min_{x \in \mathbb{Z}^k \times \mathbb{R}^{n-k}} \{c^T x \colon (a^j)^T x \leq b^j,\ \forall (a^j, b^j) \in \{(\bar{a}^j, \bar{b}^j) + \alpha u : u \in \mathcal{U}\}, j \in J\}, \quad (\mathrm{PR}_\alpha)$$

whereby $\mathcal{U} \subseteq \mathbb{R}^{n+1}$ is a convex and compact uncertainty set. In analogy to [19, 22, 23, 29], we further assume that the uncertainty set $\mathcal{U}$ contains zero in its interior.

Assumption 1. Uncertainty set $\mathcal{U}$ includes zero in its interior, i.e., $0 \in \operatorname{int} \mathcal{U}$ holds.

This implies that the uncertainty set $\mathcal{U}$ is full-dimensional, i.e. every variable is affected by uncertainties. We note that one can transform a robust optimization problem with an uncertainty set that does not contain zero to an equivalent robust problem with an uncertainty set that *contains* zero, see Chapter 1 of the book [3]. It is, however, not possible to guarantee that zero is *in the interior* of the uncertainty set $\mathcal{U}$. This is the case, for instance, if one variable is not affected by uncertainty, i.e., the projection of $\mathcal{U}$ on a single variable is just the set containing only zero. Furthermore, we note that the standard transformation of the uncertainty set does not maintain the form of (PR_α).

Assumption 1 guarantees that the radius of robust feasibility of LPs is finite, as shown in [23]. Additionally, we assume that the nominal problem (PR_0) is feasible, i.e., $\{x \in \mathbb{Z}^k \times \mathbb{R}^{n-k} \colon \bar{a}^j x \leq \bar{b}^j, j \in J\} \neq \emptyset$. Following the notion of [19, 23], who consider the radius of robust feasibility for linear problems, we define the *radius of robust feasibility* (RRF) for the parametric uncertain mixed-integer problem (P) as

$$\rho_{\mathrm{MIP}} := \sup\{\alpha \geq 0 \colon (\mathrm{PR}_\alpha) \text{ is feasible}\}.$$

The definition of the RRF ρ_{MIP} does not necessarily imply the feasibility of ($\mathrm{PR}_{\rho_{\mathrm{MIP}}}$), even in the case of linear problems, see Example 2.2 in [23]. If ($\mathrm{PR}_{\rho_{\mathrm{MIP}}}$) is feasible, we say that the RRF is attained, otherwise it is not attained. Proposition 2.3 in [23] states a sufficient condition so that the RRF is attained by a feasible solution.

We note that (PR_α) is a semi-infinite MIP that consists of infinitely many constraints and finitely many variables. Thus, it cannot easily be solved by known techniques. We now reformulate (PR_α) with the help of Fenchel duality in order to obtain an ordinary robust counterpart, i.e., the robust counterpart consists of finitely many variables and constraints. For ease of notation, we use index set $I := \{1, ..., n\}$ and $b := n + 1$ in the remainder of this paper. We further introduce the indicator function $\delta(x \mid \mathcal{U})$ for $x \in \mathbb{R}^{n+1}$, which evaluates to zero if $x \in \mathcal{U}$ holds and otherwise to $+\infty$. Moreover, let $\delta^\star(y \mid \mathcal{U}) = \sup_{u \in \mathcal{U}} y^T u$ denote the conjugate function of the indicator function, which is also called support function.

Proposition 2.1. *Let $\alpha \geq 0$ be fixed. Then, the feasible region of* (PR_α) *equals the feasible region of the ordinary counterpart*

$$\{x \in \mathbb{Z}^n \times \mathbb{R}^{n-k} \mid (\bar{a}^j)^T x + \alpha \delta^\star((x, -1)^T \mid \mathcal{U}) \leq \bar{b}^j, j \in J\}. \quad (1)$$

Proof. The claim follows from Theorem 2 in [4] and the positive homogeneity of $\delta^\star(y \mid \mathcal{U})$. ☐

Consequently, we obtain

$$\min_{x \in \mathbb{Z}^k \times \mathbb{R}^{n-k}} \{c^T x \colon (\bar{a}^j)^T x + \alpha \delta^\star((x, -1)^T \mid \mathcal{U}) \leq \bar{b}^j, j \in J\}. \quad (\mathrm{PRC}_\alpha)$$

as the ordinary robust counterpart of (PR_α).

In general, for fixed $\alpha \geq 0$, problem (PRC_α) is a convex constrained mixed-integer problem. This holds, because for a convex and compact set $\mathcal{U}$ the support function $\delta^\star(y \mid \mathcal{U})$ is convex in y, see [9]. For many uncertainty sets $\mathcal{U}$ such as boxes, balls, cones, polyhedrals, or convex functions, an explicit formulation of (PRC$_\alpha$), especially the computation of the support function, can be found in [4].

All existing techniques for computing the RRF of continuous problems, such as [18, 19, 22, 23, 29], are based on concepts that are not transferable to MIPs. Hence, we now analyze relations about the RRF of (P) and of its LP relaxation

$$\min_{x\in\mathbb{R}^n}\{c^Tx\colon (\bar{a}^j)^Tx \le \bar{b}^j, j\in J\}. \tag{LP}$$

The robust counterpart for the uncertain linear problem (LP) with uncertainty set $\alpha\mathcal{U} \subseteq \mathbb{R}^{n+1}$ and its ordinary reformulation equal the continuous relaxations of (PR$_\alpha$) and (PRC$_\alpha$). We denote them by

$$\min_{x\in\mathbb{R}^n}\{c^Tx\colon (a^j)^Tx \le b^j,\ \forall (a^j,b^j)\in\{(\bar{a}^j,\bar{b}^j)+\alpha u : u\in\mathcal{U}\}, j\in J\}, \tag{LPR$_\alpha$}$$

$$\min_{x\in\mathbb{R}^n}\{c^Tx\colon (\bar{a}^j)^Tx + \alpha\delta^\star((x,-1)^T\mid\mathcal{U}) \le \bar{b}^j, j\in J\}. \tag{LPRC$_\alpha$}$$

We first prove some basic results, which show among other things that the RRF of (LP) is always an upper bound for ρ_{MIP}.

Theorem 2.2. *Let ρ_{MIP} be the RRF of (P). The RRF of its continuous relaxation (LP) is denoted by ρ_{LP}. Then, the following statements hold:*

(i) $0 \le \rho_{\text{MIP}} \le \rho_{\text{LP}}$.
(ii) RRF ρ_{MIP} is finite.

Proof. Each feasible solution of a MIP is feasible for its LP relaxation. Thus, the RRF of (LP) is always an upper bound for the corresponding RRF of (P). Furthermore, the RRF of an LP is finite if $0 \in \operatorname{int}\mathcal{U}$ holds, see [23]. Consequently, the RRF of (P) is finite as well. □

Next, we state a monotonicity fact regarding the feasibility of (PR$_\alpha$). It is based on the observation that if a robust optimization problem is feasible, then so is the same problem for a subset of the uncertainty set.

Observation 2.3. If x is a feasible solution to (PR$_\alpha$), then x is also feasible for (PR$_{\alpha'}$) for all $\alpha' \in [0,\alpha]$.

We now show with the help of an example that the RRF of (P) and of its LP relaxation (LP) are not necessarily equal.

Example 2.4. The constraints of the nominal problem are given by

$$-2x_1 \le -1.5,\ 2x_1 \le 3.5,\ x_1\in\mathbb{Z}, \tag{2}$$

with uncertainty set $\mathcal{U} := [-1,1]^2$. Since

$$\delta^\star((x_1,-1)\mid[-1,1]^2) = \max_{u_1,u_2\in[-1,1]}(u_1x_1-u_2) = |x_1|+1$$

holds, Proposition 2.1 leads to the following robust counterpart of (2)

$$-2x_1+\alpha|x_1| \le -1.5-\alpha,\ 2x_1+\alpha|x_1|\le 3.5-\alpha,\ x_1\in\mathbb{Z}. \tag{3}$$

The only feasible solution for the nominal problem (2) is $x_1 = 1$. Further, $x_1 = 1$ is feasible to (3) if and only if $\alpha\in[0,0.25]$ holds. Consequently, the RRF of (2) equals 0.25. Now, we consider the LP relaxation of (2). The corresponding robust counterpart equals the relaxation of (3). If x_1 is a feasible solution of the relaxation of (3), then it is a feasible solution of (2). Consequently, $0.75\le x_1\le 1.75$ holds. Since $x_1>0$, one has

$$\frac{1.5+\alpha}{2-\alpha} \le x_1 \le \frac{3.5-\alpha}{\alpha+2}$$

which entails $\alpha \le \frac{4}{9}$. Conversely, if $0\le\alpha\le\frac{4}{9}$, then every x_1 satisfying the previous inequalities is a feasible solution of the relaxation of (3). Thus, the RRF of the relaxation is $\frac{4}{9}$ that is attained by $x_1 = 1.25$. We note that the RRF of (2) and its relaxation are attained, i.e., $(\mathrm{PR}_{0.25})$ and $(\mathrm{LPR}_{\frac{4}{9}})$ are feasible.

This leads to the following.

Observation 2.5. Let ρ_{MIP} be the RRF of (P) and ρ_{LP} the RRF of its LP relaxation (LP). MIPs with $\rho_{\mathrm{MIP}} < \rho_{\mathrm{LP}}$ exist.

We now state the main result of this section, namely that if ρ_{LP} is not attained, then (P) and (LP) have the same RRF. This result provides sufficient conditions such that the RRF of a MIP can be computed by the RRF of the LP relaxation. In detail, we first compute the RRF of the LP relaxation with known techniques. If this RRF is not attained, then it is also the RRF of the corresponding MIP. Otherwise, we obtain an upper bound which is useful for computing the RRF as we will see in Section 4. Additionally, we show that a similar connection between the RRF of a MIP and its LP relaxation is not necessarily given if ρ_{LP} is attained. These findings are summarized in the next theorem.

Theorem 2.6. *Let ρ_{MIP} be the RRF of* (P) *and ρ_{LP} the RRF of its LP relaxation* (LP)*. Then, the following statements hold:*

(i) If the RRF of (LP) *is not attained, then $\rho_{\mathrm{MIP}} = \rho_{\mathrm{LP}}$ holds.*
(ii) If the RRF of (P) *is attained, then the RRF of* (LP) *is also attained.*
(iii) MIPs exist such that the RRF ρ_{LP} is attained and ρ_{MIP} is attained.
MIPs exist such that the RRF ρ_{LP} is attained and ρ_{MIP} is not attained.

We will now present several examples and lemmas. With their help, we will prove Theorem 2.6 at the end of this section.

In general, the RRF is not necessarily attained by a feasible solution. If (P) and (LP) have the same RRF and $(\mathrm{PR}_{\rho_{\mathrm{MIP}}})$ is feasible, then the RRF of (LP) is also attained because each feasible solution of $(\mathrm{PR}_{\rho_{\mathrm{MIP}}})$ is also feasible to $(\mathrm{LPR}_{\rho_{\mathrm{LP}}})$. A reversal of this relation is not true in general. That means, if the RRF of (LP) is attained, then $(\mathrm{PR}_{\rho_{\mathrm{MIP}}})$ is not necessarily feasible. We show this with the help of the following example.

Example 2.7. The constraints of the nominal problem are given by

$$-x_1 - 2x_2 \le 0.5,\ \ -x_1 + 2x_2 \le 2.5,\ \ x_1, x_2 \in \mathbb{Z}, \tag{4}$$

with uncertainty set $\mathcal{U} := [-1, 1]^3$. From Proposition 2.1 the robust counterpart of (4) reads as

$$-x_1 + \alpha|x_1| - 2x_2 + \alpha|x_2| \le 0.5 - \alpha, \tag{5a}$$

$$-x_1 + \alpha|x_1| + 2x_2 + \alpha|x_2| \le 2.5 - \alpha,\ \ x_1, x_2 \in \mathbb{Z}. \tag{5b}$$

For $\alpha \in [0, 1)$, we set $x_2 = 0$ and $(-1+\alpha) < 0$ holds. Consequently, $(x_1, 0)$ is feasible for (5) whenever $x_1 \in \mathbb{N}$ satisfies $x_1 \ge \frac{0.5-\alpha}{\alpha-1}$. Thus, the RRF of (4) is at least 1. We now consider $\alpha = 1$. Since $-x_1 + \alpha|x_1| \ge 0$ holds for every $x_1 \in \mathbb{R}$, it follows $x_2 > 0$ by (5a). Consequently, from (5) we obtain $-x_2 \le -0.5$ and $3x_2 \le 1.5$ that has to be satisfied by an integer solution which leads to a contradiction. Consequently, the RRF of (4) equals 1 due to Observation 2.3 and further it is not attained. We now consider the relaxation of (4), i.e., $x_1, x_2 \in \mathbb{R}$. Its robust counterpart equals the relaxation of (5). Then, $x_1 = 0, x_2 = 0.5$ is a feasible solution for $\alpha \in [0, 1]$ of the corresponding robust counterpart. For $\alpha > 1$ the inequality $-x_1 + \alpha|x_1| \ge 0$ holds for $x_1 \in \mathbb{R}$ and thus, from (5a) it follows $x_2 > 0$. Consequently, we obtain from (5) the inequalities $-x_2 < -0.5$ and $x_2 < 0.5$ that have to be satisfied, which is a contradiction. Thus, the RRF of the relaxation of (4) equals 1 and it is attained.

If we slightly increase the right-hand side of (4), then we obtain the same result that ($\text{LPR}_{\rho_{\text{LP}}}$) is feasible and ($\text{PR}_{\rho_{\text{MIP}}}$) is infeasible, but this time $\rho_{\text{MIP}} < \rho_{\text{LP}}$ holds. An example for this adaption is given as follows.

Example 2.8. The constraints of the nominal problem are given by

$$-x_1 - 2x_2 \leq 0.6,\ -x_1 + 2x_2 \leq 2.6,\ x_1, x_2 \in \mathbb{Z}.$$

Then, the RRF of (P) equals 1 and it is not attained. The RRF of (LP) equals $\frac{16}{15}$ that is attained by $x_1 = 0, x_2 = 0.5$.

We now show several statements that lead to the proof of the main result (i) of Theorem 2.6. The latter says that if (LP) does not attain its RRF, then (P) and (LP) have the same RRF. We first prove that if the RRF ρ_{MIP} is not attained, then an unbounded sequence of solutions exists such that for every $\alpha < \rho_{\text{MIP}}$ an element of the sequence solves (PRC_α).

Lemma 2.9. *If the RRF ρ_{MIP} of* (P) *is not attained, then a positive and strictly increasing sequence $(\alpha^l)_{l\in\mathbb{N}}$ and an unbounded sequence in $\mathbb{R}^n$, $(x^l)_{l\in\mathbb{N}}$, exist such that $(\alpha^l)_{l\in\mathbb{N}}$ converges to ρ_{MIP} and x^l is feasible to* (PRC_{α^l}) *for all $l \in \mathbb{N}$.*

Proof. Since (P) is feasible and ρ_{MIP} is not attained, $\rho_{\text{MIP}} > 0$ holds. Consequently, a positive and strictly increasing sequence $(\alpha^l)_{l\in\mathbb{N}}$ that converges to ρ_{MIP} exists. Furthermore, a sequence in $\mathbb{R}^n$, $(x^l)_{l\in\mathbb{N}}$, exists such that x^l is feasible to (PRC_{α^l}) for all $l \in \mathbb{N}$. We now have to show that the sequence $(x^l)_{l\in\mathbb{N}}$ is unbounded. To this end, we contrarily assume that $(x^l)_{l\in\mathbb{N}}$ is bounded. Consequently, and by passing to a subsequence if necessary, we may assume that $x^l \longrightarrow \bar{x}$ holds, with $\bar{x}_i \in \mathbb{Z}$ for $i = 1, \dots, k$ thanks to the closedness of $\mathbb{Z}$. Considering (PRC_{α^l}) together with a solution x^l for an arbitrary $j \in J$ leads to

$$(\bar{a}^j)^T x^l + \alpha^l \delta^\star((x^l, -1)^T \mid \mathcal{U}) \leq \bar{b}^j. \tag{6}$$

Passing to the limit in (6), we obtain

$$(\bar{a}^j)^T \bar{x} + \rho_{\text{MIP}} \delta^\star((\bar{x}, -1)^T \mid \mathcal{U}) \leq \bar{b}^j.$$

Thus, $\bar{x}$ is a feasible solution to ($\text{PRC}_{\rho_{\text{MIP}}}$), which contradicts the requirements. $\square$

We next prove that under the given conditions we can arbitrarily expand the slack of any constraint of (PR_{α^l}).

Lemma 2.10. *Let $(\alpha^l)_{l\in\mathbb{N}}$ be a strictly increasing positive sequence and an unbounded sequence in $\mathbb{R}^n$, $(x^l)_{l\in\mathbb{N}}$, exist such that x^l is feasible to* (PR_{α^l}) *for all $l \in \mathbb{N}$. Then, for an arbitrary value $M \geq 0$ and index $\hat{l} \in \mathbb{N}$ there exists an index $\bar{l} > \hat{l}$ such that for all $u = \binom{u_I}{u_b} \in \mathcal{U}$, $j \in J$, and $l \geq \bar{l}$ the inequality*

$$(\bar{a}^j)^T x^l + \alpha^{\hat{l}}(u_I^T x^l - u_b) + M \leq \bar{b}^j$$

holds.

Proof. For a sufficiently small number $\beta > 0$, we know that $\pm\beta e_v \in \mathcal{U}$ for $v \in I$ holds, whereby e_v is the vth unit vector of $\mathbb{R}^{n+1}$, because $0 \in \text{int}\, \mathcal{U}$. Passing to a subsequence if necessary, we know that $v \in I$ with $|x_v^l| \longrightarrow +\infty$ exists because the sequence $(x^l)_{l\in\mathbb{N}}$ is unbounded. We can assume w.l.o.g. that $x_v^l \longrightarrow +\infty$ holds due to $\pm\beta e_v \in \mathcal{U}$. Additionally, we can assume that $(x_v^l)_{l>\hat{l}}$ is strictly increasing and we know that $(\alpha^l)_{l\in\mathbb{N}}$ is strictly increasing. Consequently, an index $\bar{l}$ exists such that for all $l \geq \bar{l}$ the inequality $(\alpha^l - \alpha^{\hat{l}})\beta x_v^l \geq M$ holds. We now choose an arbitrary index $j \in J$, $u \in \mathcal{U}$, and consider $l > \bar{l}$. From the convexity of $\mathcal{U}$ it follows $u' := \frac{\alpha^{\hat{l}}}{\alpha^l} u + (1 - \frac{\alpha^{\hat{l}}}{\alpha^l})\beta e_v \in \mathcal{U}$. The element x^l is a feasible solution to (PR_{α^l}). Hence,

$$(\bar{a}^j)^T x^l + \alpha^l((u_I')^T x^l - u_b') = (\bar{a}^j)^T x^l + \alpha^{\hat{l}}(u_I^T x^l - u_b) + (\alpha^l - \alpha^{\hat{l}})\beta x_v^l \leq \bar{b}^j \tag{7}$$

is satisfied for every $l > \bar{l}$. The inequality $(\alpha^l - \alpha^{\hat{l}})\beta x_v^l \geq M$, which is independent from the chosen u, holds and thus, (7) shows the claim. □

Due to the compactness of $\mathcal{U}$, we know that rounding down any solution leads to a bounded difference in the left side of any constraint in (PRC_α). For $x \in \mathbb{R}^n$, $\lfloor x \rfloor$ denotes the vector whose vth component is the lower integer part of x_v.

Lemma 2.11. *For fixed $\alpha \geq 0$, a positive value $M > 0$ exists such that the inequalities*

$$|(\bar{a}^j)^T(x - \lfloor x \rfloor) + \alpha u_I^T(x - \lfloor x \rfloor)| \leq M \tag{8}$$

are satisfied for any $u \in \mathcal{U}$, $x \in \mathbb{R}^n$, and $j \in J$.

Finally, we can prove Theorem 2.6.

Proof of Theorem 2.6. Examples 2.4, 2.7, and 2.8 show Statement (iii).

We now prove Statement (i). To this end, we assume w.l.o.g. that ρ_{LP} is positive. The RRF ρ_{LP} is not attained and hence, from Lemma 2.9 it follows that a strictly increasing positive sequence $(\alpha^l)_{l \in \mathbb{N}}$ with $0 < \alpha^l < \rho_{\text{LP}}$ and an unbounded sequence in $\mathbb{R}^n$, $(x^l)_{l \in \mathbb{N}}$, exist such that α^l converges to ρ_{LP} and x^l is feasible to (LPR_{α^l}) for all $l \in \mathbb{N}$. For an arbitrary fixed index $\hat{l} \in \mathbb{N}$, we now construct a solution $\hat{x}^{\hat{l}}$ that is feasible to ($\text{PR}_{\alpha^{\hat{l}}}$). Due to Lemma 2.11, we can choose $M > 0$ such that (8) is satisfied. We now apply Lemma 2.10 for this value M. Consequently, a solution x^l exists such that the inequalities

$$(\bar{a}^j)^T x^l + \alpha^{\hat{l}}(u_I^T x^l - u_b) + M \leq \bar{b}^j, \qquad u \in \mathcal{U},\ j \in J, \tag{9}$$

are satisfied. For an arbitrary element $u \in \mathcal{U}$ and $j \in J$, the inequalities

$$\begin{aligned}
\bar{b}^j &\geq (\bar{a}^j)^T x^l + \alpha^{\hat{l}}(u_I^T x^l - u_b) + M \\
&= (\bar{a}^j)^T \lfloor x^l \rfloor + \alpha^{\hat{l}}(u_I^T \lfloor x^l \rfloor - u_b) + (\bar{a}^j)^T(x^l - \lfloor x^l \rfloor) + \alpha^{\hat{l}} u_I^T(x^l - \lfloor x^l \rfloor) + M \\
&\geq (\bar{a}^j)^T \lfloor x^l \rfloor + \alpha^{\hat{l}}(u_I^T \lfloor x^l \rfloor - u_b),
\end{aligned}$$

follow from (8) and (9). Thus, $\hat{x}^{\hat{l}} := \lfloor x^l \rfloor$ is an integer solution to ($\text{PR}_{\alpha^{\hat{l}}}$). We have arbitrarily chosen $\hat{l} \in \mathbb{N}$ and hence, we can construct for each $\hat{l} \in \mathbb{N}$ an integer solution which is feasible for ($\text{PR}_{\alpha^{\hat{l}}}$). This, the convergence of $(\alpha^{\hat{l}})_{\hat{l} \in \mathbb{N}}$ to ρ_{LP}, and Statement (i) of Theorem 2.2, prove that $\rho_{\text{MIP}} = \rho_{\text{LP}}$ holds.

We now show Statement (ii). We contrarily assume that the RRF of (LP) is not attained. Thus, $\rho_{\text{MIP}} = \rho_{\text{LP}}$ follows from Statement (i) of Theorem 2.6. Due to the requirements, ($\text{PR}_{\rho_{\text{MIP}}}$) is feasible, which is a contradiction to the assumption, because each feasible solution of ($\text{PR}_{\rho_{\text{MIP}}}$) is feasible to ($\text{LPR}_{\rho_{\text{LP}}}$). □

The proof of this theorem closes the section. We will extend our investigations to linear optimization problems that contain safe constraints and variables in the following section.

3. Extension of the RRF to Include Safe Constraints and Variables

As mentioned in the introduction, there is a need to integrate safe variables and constraints into the concept of the RRF since often only parts of optimization models are affected by uncertainty in practice. Thus, a full-dimensional uncertainty set $\mathcal{U}$ with $0 \in \text{int}\, \mathcal{U}$ such as in Assumption 1 is not given in this context. Consequently, many known techniques for computing the RRF of LPs such as in [18, 19, 22, 23, 29] are not applicable anymore. Moreover, it is sometimes necessary to choose different not necessarily full-dimensional uncertainty sets for different constraints. In this case, the setting of Section 2, in which we consider in line with the common literature the same full-dimensional uncertainty set $\mathcal{U}$ for all constraints, is not suitable.

Additionally, a general weakness of the common definition of the RRF in view of comparing the RRF for different models of the same problem is that scaling the constraints of the nominal problem (P) changes the RRF, which can make the RRF values meaningless in practice. We illustrate this by the following example.

Example 3.1. We consider the uncertainty set $\mathcal{U} = [-1, 1]^2$. Then, a nominal problem with constraints given by $-x_1 \le 1,\ x_1 \in \mathbb{R}$, has RRF 1 whereas scaling this nominal problem by a factor of 2 leads to $-2x_1 \le 2,\ x_1 \in \mathbb{R}$, with RRF 2.

The latter example and the above mentioned limitations of the setting for the RRF from Section 2 motivate us to extend this setting. This will allow us to apply the concept of the RRF to more MIP instances and applications such as computing the "most robust" solution in robust facility location design.

We now introduce our extended setting for the RRF of a MIP. In analogy to Section 2, we consider the nominal MIP (P). Let $\alpha \ge 0$ be a fixed value and μ^j the smallest absolute nonzero coefficient of the jth constraint of (P). The robust counterpart for the uncertain MIP (P) with uncertainty sets $\alpha\bar{\mathcal{U}}_j, j \in J$, is now given by

$$\min_{x \in \mathbb{Z}^k \times \mathbb{R}^{n-k}} \{c^T x \colon (a^j)^T x \le b^j,\ \forall (a^j, b^j) \in \{(\bar{a}^j, \bar{b}^j) + \alpha u : u \in \bar{\mathcal{U}}_j\}, j \in J\}, \quad (\mathrm{EPR}_\alpha)$$

whereby for $j \in J$ the uncertainty set $\bar{\mathcal{U}}_j := \mu^j\, \mathcal{U}_j \subset \mathbb{R}^{n+1}$ is composed of a convex and compact set $\mathcal{U}_j$ that is scaled by μ^j. In contrast to (PR_α) of Section 2, we now consider in (EPR_α) for every constraint an own uncertainty set. These sets are not necessarily equal. Additionally, for $j \in J$ every uncertainty set $\bar{\mathcal{U}}_j$ is scaled by the smallest absolute nonzero coefficient of the jth constraint. The latter prevents that the RRF of a MIP can be increased by scaling the nominal problem such as in Example 3.1, which we will show later in this section, see Lemma 3.6. We note that the uncertain problem (PR_α) of the previous section is a special case of the extended uncertain problem (EPR_α).

In contrast to the setting of Section 2 that requires zero in the interior of the uncertainty set, see Assumption 1, we relax this condition such that zero is only a part of our uncertainty set. Consequently, the uncertainty set is not necessarily full-dimensional and we now can model safe variables and constraints. A variable $x_i, i \in I$, is said to be safe for the jth constraint, $j \in J$, if the projection of $\bar{\mathcal{U}}_j$ on the ith axis equals $\{0\}$. Further, a variable $x_i, i \in I$, is said to be safe if it is safe for each constraint $(\bar{a}^j)^T x \le \bar{b}^j, j \in J$.

For constraints, we now differentiate between two notions of being safe. A constraint $(\bar{a}^j)^T x \le \bar{b}^j, j \in J$, is *syntactically* safe if $\bar{\mathcal{U}}_j = \{0\}$. It is *semantically* safe, if $\delta^\star((x, -1)^T \mid \bar{\mathcal{U}}_j) = 0$ for all feasible points $x \in \mathbb{R}^n$ of (P). Whereas a syntactically safe constraint is also semantically safe, the converse statement is not necessarily true.

Considering the input data of the optimization problem, we can easily check whether a constraint is syntactically safe but not whether it is semantically safe. We note that decision makers can explicitly model syntactically safe constraints by setting the corresponding uncertainty set to zero. Throughout the following sections, we use safe as short form of semantically safe, if not explicitly stated otherwise.

The requirement that the uncertainty set contains zero is reasonable because it ensures that the nominal problem (EPR_0) is feasible for the RRF.

Assumption 2. Zero is contained in every uncertainty set $\bar{\mathcal{U}}_j$ for $j \in J$.

In analogy to Section 2, we define the *radius of robust feasibility* (RRF) of a given MIP in our extended setting by

$$\rho_{\mathrm{MIP}} := \sup\{\alpha \ge 0 \colon (\mathrm{EPR}_\alpha) \text{ is feasible}\}.$$

Similar to Proposition 2.1, we reformulate the feasible region of the semi-infinite problem (EPR_α) and obtain the ordinary robust counterpart

$$\min_{x \in \mathbb{Z}^k \times \mathbb{R}^{n-k}} \{c^T x \colon (\bar{a}^j)^T x + \alpha \delta^\star((x, -1)^T \mid \bar{\mathcal{U}}_j) \le \bar{b}^j, j \in J\}. \qquad (\mathrm{EPRC}_\alpha)$$

In analogy to Section 2, the robust counterparts corresponding to the continuous relaxation of (EPR_α) equal the continuous relaxation of (EPRC_α). We note that the setting of Section 2 is included in our extended setting of this section. We now compare the two settings and highlight similarities and differences.

First, we summarize all statements of Section 2 that are satisfied in our extended setting and can be shown analogously to the previous section.

Observation 3.2. Let ρ_{MIP} be the RRF of (P) and ρ_{LP} the RRF of its LP relaxation (LP). Then, the following statements hold:

(i) $0 \le \rho_{\mathrm{MIP}} \le \rho_{\mathrm{LP}}$.
(ii) MIPs with $\rho_{\mathrm{MIP}} < \rho_{\mathrm{LP}}$ exist.
(iii) MIPs exist such that the RRF ρ_{LP} is attained and ρ_{MIP} is attained.
MIPs exist such that the RRF ρ_{LP} is attained and ρ_{MIP} is not attained.

We also note that Observation 2.3 and Lemma 2.9 are valid in our new setting, which can be shown in analogy to Section 2.

We now turn to the differences between the two considered settings for the RRF. Using counterexamples we show that several statements of the previous Section 2 are not satisfied in our extended setting. Especially, the main result, Statement (i) of Theorem 2.6, is not satisfied anymore. First, we note that the RRF is not necessarily finite in our new setting, which especially holds for every feasible nominal problem (P) if the uncertainty set contains only zero.

Observation 3.3. MIPs exist such that the RRF of (P) is infinite.

The next example shows that if the RRF ρ_{LP} of the LP relaxation (LP) is not attained, then the RRF ρ_{MIP} of (P) is not necessarily equal to ρ_{LP}.

Example 3.4. The constraints of the nominal problem are given by

$$x_1 \le 1, \ -x_1 \le 0.1, \ -x_2 \le -2, \ x_1 \in \mathbb{Z}, x_2 \in \mathbb{R}, \qquad (10)$$

with the uncertainty sets $\bar{\mathcal{U}}_1 = [0]^2 \times [-0.5, 0.5]$, $\bar{\mathcal{U}}_2 = 0.1 \cdot ([0]^2 \times [-5, 5])$, and $\bar{\mathcal{U}}_3 = [0] \times [-1, 1] \times [0]$. Proposition 2.1 leads to the robust counterpart of (10)

$$x_1 \le 1 - 0.5\alpha, \ -x_1 \le 0.1 - 0.5\alpha, \ -x_2 + \alpha |x_2| \le -2, \ x_1 \in \mathbb{Z}, x_2 \in \mathbb{R}. \qquad (11)$$

From Counterpart (11) it follows that the RRF ρ_{MIP} of (10) equals 0.2 and it is attained by any point $(0, x_2)$ such that $x_2 \ge 2.5$.

We now consider the LP relaxation of (10) and the corresponding counterpart, which is the continuous relaxation of (11). For every $\alpha \in [0, 1)$ the element $(x_1, x_2) = (0.5, 2/(1-\alpha))$ is feasible for the continuous robust counterpart. Furthermore, for $\alpha = 1$ the corresponding counterpart is infeasible because $-x_2 + |x_2| \le -2, \ x_2 \in \mathbb{R}$, cannot be satisfied. Consequently, the RRF ρ_{LP} of the LP relaxation of (10) equals 1 and is not attained by a feasible solution.

From Example 3.4 it follows that the main result of Section 2, Statement (i) of Theorem 2.6, is not valid in our new setting for the RRF. Furthermore, Statement (ii) of Theorem 2.6 does not hold.

Lemma 3.5. *Let ρ_{MIP} be the RRF of* (P) *and ρ_{LP} the RRF of its LP relaxation* (LP)*. Then, the following statements hold:*

(i) MIPs exist such that ρ_{LP} is not attained and $\rho_{\mathrm{MIP}} < \rho_{\mathrm{LP}}$ holds.
(ii) MIPs exist such that the RRF ρ_{MIP} is attained and ρ_{LP} is not attained.

In addition that we can now handle safe constraints and variables in our extended setting, we now prove that scaling the nominal problem by a positive factor does not change the RRF, which is not valid for the RRF in the setting of Section 2, see Example 3.1.

Lemma 3.6. *Let ρ_{MIP} be the RRF of* (P) *and $\lambda^j > 0, j \in J$, positive factors. Then, ρ_{MIP} is also the RRF of the λ-scaled problem* (P)*, i.e., ρ_{MIP} is the RRF of*

$$\min_{x \in \mathbb{Z}^k \times \mathbb{R}^{n-k}} \{c^T x \colon \lambda^j (\bar{a}^j)^T x \leq \lambda^j \bar{b}^j, j \in J\}. \tag{12}$$

Proof. For every $j \in J$, scaling the jth constraint of the nominal problem (P) by λ^j also scales the smallest absolute nonzero coefficient μ^j of the jth constraint by λ^j. Hence, for $j \in J$ the uncertainty set $\bar{\mathcal{U}}_j$ is scaled by λ^j. From this it follows that the uncertain problem of (12) equals (EPR_α). Thus, ρ_{MIP} is also the RRF of (12). □

We now have analyzed similarities and differences for the setting of the RRF in Section 2 and our extended setting. To conclude this section, we present a necessary optimality condition for the RRF of a MIP in our extended setting that we then extend to a necessary and sufficient condition under additional assumptions. Its basic idea is rather simple, if none of the constraints is tight for a considered feasible solution, then we can increase the uncertainty set which implies that the chosen size of the uncertainty set was not maximal.

Theorem 3.7. *Let $\alpha \geq 0$ be the finite RRF of* (P)*. Then, for every feasible solution $x \in \mathbb{Z}^k \times \mathbb{R}^{n-k}$ of* (EPRC_α) *there exists an index $j \in J$ which satisfies*

$$(\bar{a}^j)^T x + \alpha \delta^\star((x, -1)^T \mid \bar{\mathcal{U}}_j) = \bar{b}^j.$$

Proof. Let $\alpha \in \mathbb{R}$ be the finite RRF of (P). We contrarily assume that (ε, x) with $\varepsilon > 0$ exists such that x is feasible for (EPRC_α) and

$$(\bar{a}^j)^T x + \alpha \delta^\star((x, -1)^T \mid \bar{\mathcal{U}}_j) + \varepsilon \leq \bar{b}^j, \quad j \in J \setminus S, \tag{13}$$

is satisfied, whereby $\delta^\star((x, -1)^T \mid \bar{\mathcal{U}}_j)$ is positive only for $j \in J \setminus S$. We note that $J \setminus S$ is nonempty, because the RRF is finite. Further, the support function $\delta^\star((x, -1)^T \mid \bar{\mathcal{U}}_j)$ is nonnegative because for $j \in J$ the uncertainty set $\bar{\mathcal{U}}_j$ contains zero. The inequalities

$$\alpha \leq \frac{\bar{b}^j - (\bar{a}^j)^T x - \varepsilon}{\delta^\star((x, -1)^T \mid \bar{\mathcal{U}}_j)}, \quad j \in J \setminus S$$

hold, which follows from (13). We now set

$$\alpha' = \min_{l \in J \setminus S} \frac{\bar{b}^l - (\bar{a}^l)^T x}{\delta^\star((x, -1)^T \mid \bar{\mathcal{U}}_l)}.$$

Then, $\alpha' > \alpha$ holds because ε is positive. Furthermore, for $j \in J \setminus S$ the inequality

$$(\bar{a}^j)^T x + \alpha' \delta^\star((x, -1)^T \mid \bar{\mathcal{U}}_j) \leq (\bar{a}^j)^T x \ + \frac{\bar{b}^j - (\bar{a}^j)^T x}{\delta^\star((x, -1)^T \mid \bar{\mathcal{U}}_j)} \delta^\star((x, -1)^T \mid \bar{\mathcal{U}}_j) \leq \bar{b}^j$$

is satisfied. Consequently, the solution x is feasible for ($\mathrm{EPRC}_{\alpha'}$). This shows together with Observation 2.3 that α cannot be the RRF of (P). □

In the following, the index set $S_{\mathrm{MIP}} \subseteq J$ contains all "safe" constraints, i.e., for every feasible solution x of (P) the equality $\delta^\star((x, -1)^T \mid \bar{\mathcal{U}}_j) = 0$ holds for $j \in S_{\mathrm{MIP}}$. If the RRF of a given MIP is attained and for each feasible solution x of (P) the counterpart $\delta^\star((x, -1)^T \mid \bar{\mathcal{U}}_j)$ is positive for $j \in J \setminus S_{\mathrm{MIP}}$, then the previous necessary optimality condition can be extended to a necessary and sufficient optimality condition. To this end, we introduce the optimization problem (SPRC$_\alpha$)

$$
\begin{aligned}
\sup_{x,\varepsilon} \quad & \varepsilon \\
\text{s.t.} \quad & (\bar{a}^j)^T x + \alpha \delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) + \varepsilon \le \bar{b}^j, \quad j \in J \setminus S_{\text{MIP}}, \\
& (\bar{a}^j)^T x \le \bar{b}^j, j \in S_{\text{MIP}}, \ x \in \mathbb{Z}^k \times \mathbb{R}^{n-k}, \ \varepsilon \ge 0.
\end{aligned}
\tag{SPRC$_\alpha$}
$$

Lemma 3.8. *Let ρ_{MIP} be the RRF of (P), $\alpha \ge 0$, and for every feasible solution x of (P) the inequality $\delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) > 0$ holds for $j \in J \setminus S_{MIP}$. If the optimal objective value of (SPRC$_\alpha$) is zero, then it is attained and α equals ρ_{MIP}.*

Proof. Due to the optimal objective value being zero and constraint $\varepsilon \ge 0$, Problem (SPRC$_\alpha$) is feasible and every feasible solution (ε, x) satisfies $\varepsilon = 0$. Consequently, the optimal objective value is attained. For a given $\alpha \ge 0$, let $(0, x)$ be an optimal solution of (SPRC$_\alpha$). We now assume that $\alpha \ne \rho_{\text{MIP}}$ holds. If $\alpha > \rho_{\text{MIP}}$ is satisfied, then this is a contradiction to the optimality of the RRF ρ_{MIP} due to Observation 2.3 and the feasibility of (SPRC$_\alpha$). We now assume $0 \le \alpha < \rho_{\text{MIP}}$. Consequently, α' with $0 \le \alpha < \alpha' \le \rho_{\text{MIP}}$ and a solution x' exists such that

$$(\bar{a}^j)^T x' + \alpha' \delta^\star((x',-1)^T \mid \bar{\mathcal{U}}_j) \le \bar{b}^j, \quad j \in J, \tag{14}$$

holds. Due to the requirements $\delta^\star((x',-1)^T \mid \bar{\mathcal{U}}_j) > 0$ for $j \in J \setminus S_{\text{MIP}}$ is satisfied and thus, from (14) follows

$$(\bar{a}^j)^T x' + \alpha \delta^\star((x',-1)^T \mid \bar{\mathcal{U}}_j) < \bar{b}^j, \quad j \in J \setminus S_{\text{MIP}}.$$

Consequently, the objective value of (SPRC$_\alpha$) is

$$\varepsilon = \min_{j \in J \setminus S_{\text{MIP}}} \bar{b}^j - (\bar{a}^j)^T x' - \alpha \delta^\star((x',-1)^T \mid \bar{\mathcal{U}}_j) > 0$$

for (ε, x'). This is a contradiction to the optimality of $(0, x)$ for α. Thus, $\alpha = \rho_{\text{MIP}}$ is satisfied. □

Finally, we present our necessary and sufficient optimality condition for the RRF.

Theorem 3.9. *Let the RRF ρ_{MIP} of (P) be attained, $S_{MIP} \ne J$, and for every feasible solution x of (P) the inequality $\delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) > 0$ holds for $j \in J \setminus S_{MIP}$. Then, the value α equals ρ_{MIP} if and only if the optimal objective value of (SPRC$_\alpha$) equals zero.*

Proof. The RRF is attained, i.e., (EPRC$_{\rho_{\text{MIP}}}$) is feasible. Moreover, for every feasible solution x of (P) the inequality $\delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) > 0$ holds for $j \in J \setminus S_{\text{MIP}}$ with $S_{\text{MIP}} \ne J$ and thus, the RRF is finite. Let α be equal to the RRF ρ_{MIP} and ε the optimal objective value of (SPRC$_\alpha$). Since the RRF is attained, (EPR$_\alpha$) and (SPRC$_\alpha$) are feasible. Consequently, ε cannot equal zero while being not attained. If ε is positive, then a feasible solution (ε, x) of (SPRC$_\alpha$) with $\varepsilon > 0$ exists. This is a contradiction to the optimality of α because of Theorem 3.7 and its proof. Consequently, ε equals zero and is attained by a feasible solution of (SPRC$_\alpha$). Thus, the claim is shown by Lemma 3.8. □

Theorem 3.9 is valid for the setting of Section 2 without assuming $\delta^\star((x,-1)^T \mid \mathcal{U}) > 0$ for every feasible solution x of (P) because Assumption 1 implies the latter.

We now move on to the computation of the RRF for LPs as well as MIPs including safe variables and constraints in our extended setting.

4. Computing the RRF Including Safe Constraints and Variables

Many known techniques for computing the RRF rely on full-dimensional uncertainty sets and compute the RRF for continuous problems, see [18, 19, 22, 23, 29]. Hence, it is not obvious if and how these techniques can be applied to our extended setting of Section 3 in which MIPs with different not necessarily full-dimensional uncertainty sets are considered. The latter enables us to consider MIPs including safe variables and constraints. Consequently, there is a lack of methods that compute the RRF for LPs as well as for MIPs including safe variables and constraints. This section is structured as follows. We first show a method for computing the RRF of LPs including safe variables and constraints. We then briefly show that the RRF of a bounded integer problem can be computed by solving maximally two integer problems. Finally, we present first methods for computing the RRF of MIPs in our extended setting of Section 3.

4.1. **Computing the RRF for Linear Problems.** In this subsection, we present a method for computing the RRF of (LP). To this end, we consider our general setting of Section 3. Throughout this section, we split the constraints of (LP) into "safe" constraints $S_{\text{LP}} \subseteq J$, i.e. for every feasible solution x of (LP) the equality $\delta^\star((x,-1) \mid \bar{\mathcal{U}}_j) = 0$ holds for $j \in S_{\text{LP}}$, and into "uncertain" constraints $J \setminus S_{\text{LP}}$. Additionally, we require the following assumption for the uncertainty sets.

Assumption 3. We assume for the uncertain constraints that, up to scaling, all uncertainty sets are identical, i.e., $\bar{\mathcal{U}}_j = \mu^j \ \lambda^j \ \mathcal{U} \subset \mathbb{R}^{n+1}$ for $j \in J \setminus S_{\text{LP}}$ holds whereby $\mathcal{U}$ is a convex and compact uncertainty set and λ^j is positive for $j \in J \setminus S_{\text{LP}}$.

We note that typically the uncertainty sets $\bar{\mathcal{U}}_j, j \in J$, are positive multiples of the Euclidean unit closed ball or of some cartesian product $\mathcal{U} = \prod_{i \in I}[-\delta_i, \delta_i]$, with $\delta_i \geq 0$ for all $i \in I$, which is in line with Assumption 3. Moreover, the positive homogeneity of $\delta^\star(x \mid \bar{\mathcal{U}}_j)$ for $j \in J$ and Assumption 3 lead to

$$\delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) = \mu^j \lambda^j \delta^\star((x,-1)^T \mid \mathcal{U}), \quad j \in J \setminus S_{\text{LP}}. \tag{15}$$

Thus, under Assumption 3, for all feasible points $x \in \mathbb{R}^n$ of (LP), the equality $\delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) = 0$ either holds for all $j \in J \setminus S_{\text{LP}}$ or for no index $j \in J \setminus S_{\text{LP}}$.

We note that this setting is more general than that of Section 2 because it does not require a full-dimensional uncertainty set and thus, we allow safe variables and constraints. We further consider objective functions as extended-value functions whereby we follow the extended-value definition in [27]. Consequently, if an optimization problem is infeasible, then its objective value is $+\infty$ for minimization problems, respectively $-\infty$ for maximization problems. Furthermore, $\frac{1}{+\infty} := 0$ and $\frac{1}{0} := +\infty$ hold.

We now give a derivation of our method that is based on fractional programming. We first handle the case that a feasible solution x of (LP) without uncertainty exists, i.e., $\delta^\star((x,-1)^T \mid \mathcal{U}) = 0$. Then, we consider the case that the RRF is zero. Afterward, we present a method that computes the RRF if the latter is positive. Finally, we combine these results in an algorithm that computes the RRF for LPs.

Clearly, if a feasible solution of (LP) which is not affected by any uncertainty exists, then the RRF is infinite.

Proposition 4.1. *Let $x \in \mathbb{R}^n$ be a feasible solution to* (LP) *such that the equality $\delta^\star((x,-1)^T \mid \mathcal{U}) = 0$ holds. Then, the RRF of* (LP) *is infinite.*

Next, we show that the requirement of Proposition 4.1 can be checked algorithmically. We know that $\delta^\star((\cdot,-1)^T \mid \mathcal{U}) \geq 0$ holds due to Assumption 2. Consequently, we can verify if the equation $\delta^\star((x,-1)^T \mid \mathcal{U}) = 0$ holds for any feasible solution x

of (LP) by checking the feasibility of the convex problem

$$\min_{x} \quad 0 \tag{16a}$$
$$\text{s.t.} \quad (\bar{a}^j)^T x \le \bar{b}^j \qquad \text{for all } j \in J, \tag{16b}$$
$$\delta^\star((x,-1)^T \mid \mathcal{U}) \le 0. \tag{16c}$$

Lemma 4.2. *A feasible solution x of* (LP) *with $\delta^\star((x,-1)^T \mid \mathcal{U}) = 0$ exists if and only if Problem* (16) *is feasible.*

We now assume that for every feasible solution x of the nominal problem (LP) the inequality $\delta^\star((x,-1)^T \mid \mathcal{U}) > 0$ holds, since otherwise the RRF is infinite which we can detect by the previously stated model.

Due to the definition of the RRF, the feasibility of (LP), and Assumption 3, the RRF of Problem (LP) can be computed by the nonlinear problem

$$\begin{aligned} \sup_{\alpha,x} \quad & \alpha \\ \text{s.t.} \quad & (\bar{a}^j)^T x + \alpha \mu^j \lambda^j \delta^\star((x,-1)^T \mid \mathcal{U}) \le \bar{b}^j && \text{for all } j \in J \setminus S_{\mathrm{LP}}, \\ & (\bar{a}^j)^T x \le \bar{b}^j && \text{for all } j \in S_{\mathrm{LP}}, \end{aligned}$$

which we can reformulate as

$$\sup_{x} \quad \min_{j \in J \setminus S_{\mathrm{LP}}} \frac{\bar{b}^j - (\bar{a}^j)^T x}{\mu^j \lambda^j \delta^\star((x,-1)^T \mid \mathcal{U})} \tag{17a}$$
$$\text{s.t.} \quad (\bar{a}^j)^T x \le \bar{b}^j \qquad \text{for all } j \in S_{\mathrm{LP}}. \tag{17b}$$

Problem (17) is a generalized fractional program. Additionally, for every feasible solution of the nominal problem (LP) and for every ratio in the objective function the corresponding nominator is nonnegative and concave and the denominator is positive and convex. Thus, Problem (17) has the form of a concave generalized fractional program, see [2, Chapter 7]. We now reduce Problem (17) to a concave single ratio fractional program, which then can be reformulated as a concave problem. To this end, we reformulate Problem (17) as follows

$$\sup_{x,\varepsilon,z} \quad \frac{z}{\delta^\star((x,-1)^T \mid \mathcal{U})} \tag{18a}$$
$$\text{s.t.} \quad (\bar{a}^j)^T x + \varepsilon_j \le \bar{b}^j \qquad \text{for all } j \in J \setminus S_{\mathrm{LP}}, \tag{18b}$$
$$(\bar{a}^j)^T x \le \bar{b}^j \qquad \text{for all } j \in S_{\mathrm{LP}}, \tag{18c}$$
$$\varepsilon_j \ge 0 \qquad \text{for all } j \in J \setminus S_{\mathrm{LP}}, \tag{18d}$$
$$\frac{\varepsilon_j}{\mu^j \lambda^j} \ge z \ge 0 \qquad \text{for all } j \in J \setminus S_{\mathrm{LP}}. \tag{18e}$$

We note that Problem (18) is a concave fractional program with a single ratio in the objective function. Furthermore, the RRF of (LP) is strictly positive if and only if a feasible solution (x,ε,z) of (18) with $z > 0$ exists because $\delta^\star((x,-1)^T \mid \mathcal{U}) > 0$ holds. We now assume that the variable z is positive and show that we can algorithmically check if the RRF is zero with the help of a linear problem.

$$\sup_{x,\varepsilon,z} \frac{z}{\delta^\star((x,-1)^T \mid \mathcal{U})} \quad \text{s.t.} \quad (18\text{b}) - (18\text{e}),\ z > 0. \tag{19}$$

Lemma 4.3. *Problem* (19) *is feasible if and only if the RRF of* (LP) *is strictly positive.*

Proof. Let (x,ε,z) satisfy constraints (18b)–(18e). Then, (x,ε,z) is feasible for Problem (19) if and only if $z > 0$ holds, which in turn is equivalent to the optimal value of Problem (18) being strictly positive. □

Clearly, we can check if Problem (19) is feasible by solving a linear problem.

Lemma 4.4. *Problem (19) is feasible if and only if the objective value of problem*

$$\max_{x,\varepsilon,z} \; z \quad \text{s.t.} \quad (18b) - (18e) \tag{20}$$

is positive.

Using linear Problem (20), we can detect whether the RRF of (LP) is strictly positive or zero. We now handle the case that the RRF is strictly positive. Thus, we consider the optimization problem, in which we minimize the reciprocal of the original objective function of (19)

$$\inf_{x,\varepsilon,z} \; \frac{\delta^\star((x,-1)^T \mid \mathcal{U})}{z} \quad \text{s.t.} \quad (18b) - (18e), \; z > 0. \tag{21}$$

We note that Problem (19) and (21) have the same feasible region and for every feasible solution the corresponding objective value is positive. Both problems share the same optimal solutions and the optimal values are reciprocal to each other. Throughout this section, we consider objective values in the extended-value sense.

Lemma 4.5. *Let (x,ε,z) be a feasible solution of Problem (19). Then, (x,ε,z) is an optimal solution of Problem (19), if and only if (x,ε,z) is an optimal solution of Problem (21).*

Let v and $\hat{v}$ be the optimal values of (19) and (21). Then, the equation $v = \frac{1}{\hat{v}}$ holds in the extended-value sense.

Due to Lemma 4.5, the optimal value of (21) is zero if and only if the RRF of (LP) is infinite. Problem (21) is equivalent to a concave fractional program with affine denominator. Thus, we can apply a variable transformation that was suggested by Charnes and Cooper [17] for linear fractional programs and later extended to nonlinear fractional programs by Schaible [31], see also [2] and the references therein. The transformation is given by

$$y = \begin{bmatrix} y_x \\ y_\varepsilon \\ y_z \end{bmatrix} = \frac{1}{z} \begin{bmatrix} x \\ \varepsilon \\ z \end{bmatrix}, \quad t = \frac{1}{z}. \tag{22}$$

Applying this variable transformation to Problem (21) together with Proposition 7.2 in Chapter 7 of [2] and the positive homogeneity of the support function lead us to the following lemma.

Lemma 4.6. *Let (x,ε,z) and (y,t) be given such that Transformation (22) holds. Then (x,ε,z) is feasible for Problem (21) if and only if (y,t) is feasible to problem*

$$\begin{aligned}
\inf_{y,t} \quad & \delta^\star((y_x,-t)^T \mid \mathcal{U}) && && \text{(23a)}\\
\text{s.t.} \quad & (\bar{a}^j)^T y_x + y_{\varepsilon_j} - t\bar{b}^j \le 0 && \text{for all } j \in J \setminus S_{LP}, && \text{(23b)}\\
& (\bar{a}^j)^T y_x - t\bar{b}^j \le 0 && \text{for all } j \in S_{LP}, && \text{(23c)}\\
& y_{\varepsilon_j} \ge \mu^j \lambda^j && \text{for all } j \in J \setminus S_{LP}, && \text{(23d)}\\
& t > 0. && && \text{(23e)}
\end{aligned}$$

Furthermore, the optimal values of Problems (21) and (23) are equal.

We now relax Problem (23) by requiring $t \ge 0$ instead of $t > 0$ in order to obtain the computationally tractable convex optimization problem

$$\inf_{y,t} \; \delta^\star((y_x,-t)^T \mid \mathcal{U}) \quad \text{s.t.} \quad (23b) - (23d), \; t \ge 0. \tag{24}$$

All constraints of Problem (24) are linear. Furthermore, optimizing (24) has the same computational complexity as optimizing a linear function over the given uncertainty set $\mathcal{U}$ with additional linear constraints.

We note that if Problem (23) is feasible, then the objective values of (23) and (24) are finite due to Assumption 2, which implies $\delta^\star((y_x, -t)^T \mid \mathcal{U}) \geq 0$. Further, we now prove that these objective values are equal.

Lemma 4.7. *Let Problem* (23) *be feasible. Then, the optimal values of Problems* (23) *and* (24) *are equal.*

Proof. Let v be the optimal value of Problem (23) and v_{relax} the optimal value of Problem (24). As Problem (24) is a relaxation of Problem (23), $v_{\text{relax}} \leq v$ holds.

So, assume, by contradiction, that there exists a solution (y^*, t^*) of Problem (24) with corresponding objective value v^* and $v^* < v$. Thus, $t^* = 0$ holds. As Problem (23) is feasible, there exists a feasible point $(\bar{y}, \bar{t})$ with $\bar{t} > 0$.

Now, set

$$\begin{bmatrix} y^k \\ t^k \end{bmatrix} = \frac{k-1}{k} \begin{bmatrix} y^* \\ t^* \end{bmatrix} + \frac{1}{k} \begin{bmatrix} \bar{y} \\ \bar{t} \end{bmatrix} \quad \text{for all } k \in \mathbb{N}.$$

Then, the pairs (y^k, t^k) are feasible for Problem (24) as its feasible region is convex. Since $t^k > 0$ holds, (y^k, t^k) is also feasible to (23). The objective values v^k of these solutions converge to v^* as the support function, $\delta^\star((y_x^k, -t^k)^T \mid \mathcal{U})$, is continuous. Hence, there exists a $\bar{k} \in \mathbb{N}$ such that $v^{\bar{k}} < v$ holds, which contradicts the fact that v is the optimal value of Problem (23). Consequently, the optimal values of Problem (24) and of Problem (23) are equal. □

Again, we use extended-values in this section.

Lemma 4.8. *Let Problem* (23) *be feasible and v the optimal value of* (24)*. Then, the RRF of* (LP) *is given by* $\frac{1}{v}$.

Proof. The claim follows from combining the previous Lemmas 4.7, 4.6, and 4.5. □

Using the previous results, we now state a complete procedure to compute the RRF of (LP) whereby the uncertainty sets satisfy Assumption 2 and 3.

Algorithm 1: Computing the RRF of a Linear Problem

Input: Linear Problem (LP) and uncertainty sets $\bar{\mathcal{U}}_j$ for $j \in J$.
Output: RRF of (LP).

1 **if** *Problem* (16) *is feasible* **then return** $+\infty$.
2 Solve $(x, \varepsilon, z) \leftarrow$ (20).
3 **if** $z = 0$ *holds* **then return** 0.
4 Compute optimal objective v of Problem (24).
5 **return** $\frac{1}{v}$.

Theorem 4.9. *Let the robust counterpart for the uncertain linear problem* (LP) *with uncertainty sets $\alpha\bar{\mathcal{U}}_j, j \in J$, satisfy Assumptions 2 and 3. Then, Algorithm 1 computes the RRF of* (LP)*.*

Proof. If Algorithm 1 stops in Line 1, then the RRF is infinite due to Proposition 4.1 and Lemma 4.2. If Algorithm 1 stops in Line 3, then the RRF is zero due to Lemmas 4.3 and 4.4. If Algorithm 1 stops in Line 5, then the feasibility of (23) follows from the positive objective value of (20) and Lemmas 4.4–4.6. Thus, we can apply Lemma 4.8, which proves the claim. □

In summary, we can efficiently compute the RRF of (LP) including safe variables and constraints by solving at most one linear and two convex optimization problems. Especially, solving the latter problems has the same computational complexity as optimizing a linear objective function over the given uncertainty set with additional linear constraints. In addition to the benefit for computing the RRF of LPs, the results can be used as an upper bound for the RRF of the corresponding MIPs which will be helpful for the later presented methods. We also note that under certain conditions the RRF of a MIP can be computed by the RRF of its LP relaxation, see Theorem 2.6.

4.2. **Computing the RRF of Bounded Integer Problems.** In this subsection, we briefly show that for a bounded linear integer problem we can compute its RRF in the setting of Section 3 by maximally solving two convex integer problems. The latter problems have the same complexity as solving an integer problem with linear objective function over the given uncertainty set with additional linear constraints. For the remainder of this subsection, we assume w.l.o.g. that our bounded integer problem (P) is a binary problem.

We first show that the compactness of the feasible region of (P) ensures that its RRF is either attained or infinite and the latter can be checked algorithmically. To this end, we note that Lemma 2.9 is also valid for a finite RRF in the setting of Section 3 which can be proven analogously.

Lemma 4.10. *If the feasible region of* (P) *is compact, then the corresponding RRF is either attained or infinite.*

Proof. We contrarily assume that the RRF is not attained and finite. Due to Lemma 2.9 an unbounded sequence of feasible solutions to (P) exists, which contradicts the compactness of the feasible region of (P). □

Additionally, we can detect if the RRF is infinite. In doing so, the index set S_{MIP} contains all safe constraints of (P) that are not affected by uncertainty.

Lemma 4.11. *Let the feasible region of* (P) *be compact. Then, the RRF of* (P) *is infinite if and only if the convex integer problem*

$$\min_x \ 0 \quad s.t. \quad \text{(16b)}, \ \delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) \le 0, j \in J \setminus S_{MIP}, \ x \in \{0,1\}^n, \tag{25}$$

is feasible.

Proof. We first assume that the RRF of (P) is infinite. Due to the requirements and the definition of the RRF, a positive and strictly increasing sequence $(\alpha^l)_{l\in\mathbb{N}}$ that converges to $+\infty$ exists. Furthermore, a sequence in $\mathbb{R}^n$, $(x^l)_{l\in\mathbb{N}}$, exists such that x^l is feasible to (EPRC$_{\alpha^l}$) for all $l \in \mathbb{N}$. Due to the compactness of the feasible region of (P), the sequence $(x^l)_{l\in\mathbb{N}}$ is bounded. Consequently, and by passing to a subsequence if necessary, we may assume that $x^l \longrightarrow \bar{x}$ holds. Considering (EPRC$_{\alpha^l}$) together with a solution x^l leads to the feasible inequalities

$$(\bar{a}^j)^T x^l + \alpha^l \delta^\star((x^l,-1)^T \mid \bar{\mathcal{U}}_j) \le \bar{b}^j, \quad j \in J \setminus S_{\text{MIP}}.$$

Since sequence $(x^l)_{l\in\mathbb{N}}$ is bounded, $(\alpha^l)_{l\in\mathbb{N}}$ converges to $+\infty$, and $\delta^\star((x^l,-1)^T \mid \bar{\mathcal{U}}_j)$ is nonnegative for $j \in J \setminus S_{\text{MIP}}$, it follows from the previous inequalities that for $j \in J \setminus S_{\text{MIP}}$ the support function $\delta^\star((x^l,-1)^T \mid \bar{\mathcal{U}}_j)$ converges to zero. Due to this, $x^l \longrightarrow \bar{x}$, and the continuity of $\delta^\star((x^l,-1)^T \mid \bar{\mathcal{U}}_j)$ for $j \in J \setminus S_{\text{MIP}}$, the equality $\delta^\star((\bar{x},-1)^T \mid \bar{\mathcal{U}}_j) = 0$ holds for $j \in J \setminus S_{\text{MIP}}$. Because of the compactness of the feasible region and $x^l \longrightarrow \bar{x}$, the solution $\bar{x}$ is feasible to (P). Thus, it is feasible to (25).

If Problem (25) is feasible, then from the nonnegativity of the support function $\delta^\star((\cdot,-1)^T \mid \bar{\mathcal{U}}_j)$ for $j \in J \setminus S_{\text{MIP}}$, it directly follows that the RRF is infinite. □

Due to the previous two lemmas, we can algorithmically check if the RRF of (P) is infinite. Thus, we now assume that the RRF is finite. Consequently, the RRF is attained because of Lemma 4.10 and we can compute the RRF by solving the nonlinear problem

$$\begin{aligned}
\max_{\alpha, x} \quad & \alpha && && \text{(26a)}\\
\text{s.t.} \quad & (\bar{a}^j)^T x + \delta^\star((\alpha x, -\alpha)^T \mid \bar{\mathcal{U}}_j) \leq \bar{b}^j && \text{for all } j \in J \setminus S_{\text{MIP}}, && \text{(26b)}\\
& (\bar{a}^j)^T x \leq \bar{b}^j && \text{for all } j \in S_{\text{MIP}}, && \text{(26c)}\\
& \alpha \geq 0, \ x \in \{0,1\}^n. && && \text{(26d)}
\end{aligned}$$

We can equivalently replace the nonlinear term αx in (26) by suitable Big-M constraints because the RRF of (P) is finite and x are binaries.

In summary, we can compute the RRF for bounded integer problems in the setting of Section 3 by solving (25) and (26). This method is straightforward and is mainly presented for the sake of completeness. Furthermore, preliminary computational results showed that its performance is bad in general and cannot be used for practical computations. It is also massively worse in comparison to the methods of the next section that are based on improved effective binary search algorithms.

4.3. **Computing the RRF of Mixed-Integer Problems.** In this subsection, we present different methods to compute the RRF of MIPs (P) in our extended setting of Section 3 in the case that the RRF is finite. In doing so, the presented methods share a common basic structure, see Algorithm 2. We note that the considered setting of the RRF includes safe constraints, respectively variables, and an own not necessarily full-dimensional uncertainty set for every constraint.

For the remainder of this subsection, we assume that the RRF of (P) is finite and bounded from above by $\bar{u}$. Further, we know that the RRF is bounded from below by zero. In analogy to Observation 2.3 for $\alpha \geq 0$ a monotonicity statement w.r.t. the corresponding ordinary counterpart (EPRC$_\alpha$) holds. Thus, we can apply a classic binary search (ClassicBin) on α w.r.t. (EPRC$_\alpha$) in order to find an approximation of the RRF. This approximation differs from the RRF no more than an a priori given error $\text{tol} > 0$. Binary search is already in itself an efficient algorithm. However, we show in addition that our theoretical findings on RRF can be used to even improve on binary search in practical computations.

Lemma 4.12. *Let ρ_{MIP} be the RRF of* (P). *Further, let α be the output of ClassicBin with initial lower bound zero, $\bar{u}$ an upper bound of the RRF, and the tolerance* tol. *Then,* (EPRC$_\alpha$) *is feasible, $|\rho_{\text{MIP}} - \alpha| \leq \text{tol}$ holds, and ClassicBin performs at most $\lceil \log_2(\frac{\bar{u}}{\text{tol}}) \rceil$ many iterations.*

An important benefit of this simple approach is that in each step of the binary search it is sufficient to only check the feasibility of (EPRC$_\alpha$). With the help of standard techniques of robust optimization, e.g., see [4], Problem (EPRC$_\alpha$) can be reformulated such that its computational complexity is equal to checking the feasibility of an optimization problem over the given uncertainty set with additional linear constraints.

We now improve ClassicBin by adding a scaling argument so that whenever (EPRC$_\alpha$) is feasible, we tighten the lower bound in the binary search. To this end, Algorithm 2 represents the basic structure of this scaling binary search (ScalingBin) and its explicit components are given in Table 1. Method ScalingBin still maintains the properties of ClassicBin.

Lemma 4.13. *Let ρ_{MIP} be the RRF of* (P). *Further, let α be the output of ScalingBin. Then,* (EPRC$_\alpha$) *is feasible, $|\rho_{\text{MIP}} - \alpha| \leq \text{tol}$ holds, and ScalingBin performs at most $\lceil \log_2(\frac{\bar{u}}{\text{tol}}) \rceil$ many iterations.*

Algorithm 2: Basic Algorithm

Input: Nominal problem (P), uncertainty sets $\bar{\mathcal{U}}_j$ for $j \in J$, tolerance tol > 0, RRF upper bound $\bar{u}$.

Output: RRF of (P).

```
Initialization.                     Init
while Condition do
    Update Estimate RRF.            Estim
    Solve Subproblem.               Subp
    Check Optimality.               Optim
    Update Upper Bound.             Upper
    Update Lower Bound.             Lower
return Results.
```

TABLE 1. Overview of algorithms with their specific components in Algorithm 2

<table>
<tr><th></th><th>ScalingBin</th><th>MaxScalingBin</th><th>PureScaling</th></tr>
<tr><td>Init</td><td colspan="2">$l \leftarrow 0, \;\; u \leftarrow \bar{u}$</td><td>$l \leftarrow 0$</td></tr>
<tr><td>Condition</td><td colspan="2">$|u - l| > \text{tol}$</td><td>$(\text{EPRC}_{(l+\text{tol})})$ feasible</td></tr>
<tr><td>Estim</td><td colspan="2">$\alpha \leftarrow \frac{u+l}{2}$</td><td>$\alpha \leftarrow l + \text{tol}$</td></tr>
<tr><td>Subp</td><td>$x \leftarrow (\text{EPRC}_\alpha)$</td><td colspan="2">$(\varepsilon, x) \leftarrow (\text{SPRC}_\alpha)$</td></tr>
<tr><td>Optim</td><td></td><td colspan="2">if $\varepsilon = 0$ then return $(\alpha, \mathsf{optimal})$</td></tr>
<tr><td>Upper</td><td>if (EPRC_α) infeasible then $\bar{u} \leftarrow \alpha$</td><td>if (SPRC_α) infeasible then $\bar{u} \leftarrow \alpha$</td><td></td></tr>
<tr><td>Lower</td><td colspan="3">$S_{\text{MIP}} \leftarrow \{j \in J \mid \delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) = 0\}, \;\; l \leftarrow \min_{j \in J \setminus S_{\text{MIP}}} \frac{\bar{b}^j - (\bar{a}^j)^T x}{\delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j)}$</td></tr>
<tr><td>Results</td><td>l</td><td colspan="2">$(l, \mathsf{non\ optimal})$</td></tr>
</table>

Proof. If we replace the operation Lower of ScalingBin, see Table 1, by $l = \alpha$, then ScalingBin equals a classic binary search. Thus, we have to prove that the outcome α' of Lower satisfies $\alpha \leq \alpha' \leq \bar{u}$ and that Problem $(\text{EPRC}_{\alpha'})$ is feasible. From the proof of Theorem 3.7 it follows the inequality $\alpha \leq \alpha'$ and the feasibility of Problem $(\text{EPRC}_{\alpha'})$. Consequently, $\alpha' \leq \bar{u}$ holds due to the monotonicity of (EPRC_α) w.r.t. α and $\bar{u}$ being an upper bound for ρ_{MIP}. □

We note that if the RRF is attained by the solution x in the operation Subp, then ScalingBin directly scales the lower bound l to the RRF in the operation Lower, which is shown in the following lemma.

Lemma 4.14. *Let the RRF ρ_{MIP} of (P) be attained and $0 \leq \alpha \leq \rho_{\text{MIP}}$. Additionally, let x be a feasible solution to (EPRC_α) as well as to $(\text{EPRC}_{\rho_{\text{MIP}}})$ and $S_{MIP} = \{j \in J \mid \delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) = 0\}$. Then, $\min_{j \in J \setminus S_{MIP}} \frac{\bar{b}^j - (\bar{a}^j)^T x}{\delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j)} = \rho_{\text{MIP}}$ holds.*

Proof. The claim follows in analogy to the proof of Theorem 3.7. □

We now integrate in ScalingBin the optimality condition for the RRF of Lemma 3.8 and Theorem 3.9 as an additional termination condition. Algorithm MaxScalingBin preserves the properties of ClassicBin for every feasible solution x of (P) under the additional assumption $\delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) > 0$ for $j \in J$. Furthermore, in the case that the RRF is attained MaxScalingBin immediately stops if the RRF is computed. The latter is not guaranteed in ScalingBin because it possibly has to tighten the upper bound first before it stops. In order to avoid this effect, MaxScalingBin solves Problem (SPRC_α) to optimality in every iteration whereas ScalingBin only checks the feasibility of (EPRC_α) in every iteration. We note that the computational complexities of (SPRC_α) and (EPRC_α) are equal.

Lemma 4.15. *Let the inequalities $\delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) > 0$ for $j \in J \setminus S_{MIP}$ hold for every feasible solution x of (P). Let $\rho_{\mathrm{MIP}} \in \mathbb{R}$ be the finite RRF of (P) and (α, flag) the output of MaxScalingBin. Then, (EPRC_α) is feasible. Additionally, if flag is equal to* optimal*, then $\alpha = \rho_{\mathrm{MIP}}$, otherwise, $|\rho_{\mathrm{MIP}} - \alpha| \leq tol$ holds. Furthermore, MaxScalingBin performs at most $\lceil \log_2(\frac{\bar{u}}{\mathrm{tol}}) \rceil$ many iterations.*

Proof. Problem (SPRC_α) is feasible if and only if (EPRC_α) is feasible. Consequently, if MaxScalingBin returns (α, non optimal) the claim follows from Lemma 4.13. Otherwise, the claim follows from Lemma 3.8. □

Finally, we present an approach that is similar to MaxScalingBin and needs the same assumption, i.e., the inequalities $\delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) > 0$ for $j \in J$ hold for every feasible solution x of (P). The method, given by Algorithm PureScaling, is based on computing the maximal slack in each iteration and then scaling the current value of the RRF. The main goal is that if we get close to the RRF very fast, then we can detect this without tightening the upper bound of the RRF in many iterations such as it can happen in the previous presented approaches. We note that PureScaling is not based on a binary search. Additionally, the upper bound of the RRF is only necessary to guarantee a finite runtime.

Lemma 4.16. *Let the inequalities $\delta^\star((x,-1)^T \mid \bar{\mathcal{U}}_j) > 0$ for $j \in J \setminus S_{MIP}$ hold for every feasible solution x of (P). Let (α, flag) be the output of PureScaling and $\rho_{\mathrm{MIP}} \in \mathbb{R}$ the finite RRF of (P). Then, (EPRC_α) is feasible. Additionally, if flag is equal to* optimal*, then $\alpha = \rho_{\mathrm{MIP}}$, otherwise, $|\rho_{\mathrm{MIP}} - \alpha| \leq tol$ holds. Furthermore, PureScaling performs at most $\lceil \frac{\rho_{\mathrm{MIP}}}{\mathrm{tol}} \rceil$ many iterations.*

Proof. The claim follows from Lemma 4.15 and the construction of PureScaling. □

We note that the worst-case runtime of PureScaling is inferior to the worst-case runtime of the presented approaches based on binary search. But in practice PureScaling detects faster if the computed RRF is in the a priori given tolerance than the approaches based on binary search, which we investigate experimentally in the next section.

5. Computational Results

In this section, we present a computational study for the previously described methods to compute the RRF for MIPs of the MIPLIB 2017 library, see [30]. To be more precise, we evaluate the impact of the aspects:

(a) The chosen method: We compare the bounded IP approach (26), the classic binary search, and Methods ScalingBin, MaxScalingBin, and PureScaling.
(b) The performance: We compare the runtime of every method and the corresponding number of iterations.
(c) Characterization of the instances: We analyze the instances w.r.t. their computed RRF ρ_{MIP} and the impact of the uncertainties. In particular, we compare the optimal nominal objective value to the optimal objective value of ($\mathrm{PR}_{\rho_{\mathrm{MIP}}}$). This comparison quantifies the *price of robustness*.

We implemented the algorithms in Python 3.6.5 and solved the MIPs with Gurobi 8.0.1, see [26]. All computations were executed on a 4-core machine with a Xeon E3-1240 v5 CPU and 32 GB RAM. Our test set consists of 165 instances from the MIPLIB 2017 library. Out of the entire MIPLIB 2017 library of 1065 instances, we only considered the benchmark set of 240 instances. We further excluded 38 instances that are classified as hard in the MIPLIB 2017. This guarantees that we can solve the nominal problem by state-of-the-art available programs within a reasonable runtime. Additionally, we excluded the remaining 5 infeasible instances. We next determine the types of constraints that we consider as syntactically safe, i.e., these constraints have an uncertainty set consisting only of the zero vector. First, we consider every constraint that consists just of a single variable as safe because it directly represents a lower bound of the corresponding variable. Additionally, every constraint that contains only binary variables with coefficients ± 1 is safe because these constraints usually represent combinatorial structures. Considering the latter constraints as unsafe leads to infeasibility in most of the cases, i.e., the RRF is zero. Due to the same reason, we consider equalities as safe. In doing so, we also exclude equalities that are simply rewritten as two linear inequalities. No further presolve routines for detecting implicit equalities are processed. Considering the previously mentioned constraints as safe leads to 32 instances that only contain safe constraints. Consequently, these instances are also excluded, which finally results in our test set of 165 instances.

In all computations, we used Gurobi with standard settings with the following adaptions. For all methods, we disabled dual reductions in order to have a more definitive conclusion about infeasibility of the model. For the classical binary search and ScalingBin, we set the parameter solution limit to 1 because we are only interested in the feasibility of the corresponding MIP in every iteration. In contrast to this, we solve the upcoming MIPs in every iteration of MaxScalingBin and PureScaling to optimality. In order to prevent that the extended runtime of solving these MIPs to optimality exceeds the potential benefit of maximizing the slack together with scaling the RRF, described in MaxScalingBin and PureScaling, we set the relative MIP gap to 0.5 as this value turned out to be reasonable in our preliminary computational results. We consider an absolute tolerance of 10^{-4} and set the time limit to 2 h. Furthermore, we introduced a relative tolerance of 10^{-4} as an additional termination condition in order to avoid numerical issues.

We next turn to the considered uncertainty set. We compute the RRF in the extended framework of Section 3. Consequently, the jth unsafe constraint has the uncertainty set $\bar{\mathcal{U}}_j := \mu^j\, \mathcal{U}_j \subset \mathbb{R}^{n+1}$, composed of a convex and compact set $\mathcal{U}_j$ that is scaled by the smallest absolute nonzero coefficient μ^j of the jth constraint. In our computational study, the uncertainty set $\mathcal{U}_j$ for the jth unsafe constraint is given as follows. For each variable with nonzero coefficient in the jth constraint, the uncertainty set for this variable is given by the interval $[-1, 1]$. The latter interval is also the uncertainty set of the right-hand side. If a variable has coefficient zero in the considered constraint, then it is considered safe for this constraint, i.e., its corresponding uncertainty set contains only zero. In total, the uncertainty set $\mathcal{U}_j$ is given by the corresponding cross products of intervals $[-1, 1]$ and sets $\{0\}$. For $\bar{\mathcal{U}}_j \neq \{0\}$, it follows from the the construction of $\bar{\mathcal{U}}_j$ that the $(n+1)$th unit vector of $\mathbb{R}^{n+1}$ is in $\bar{\mathcal{U}}_j$ and thus, $\delta^\star((x, -1) \mid \bar{\mathcal{U}}_j) > 0$ holds for every $x \in \mathbb{R}^n$. Consequently, each constraint with uncertainty set unequal to zero is (semantically) unsafe.

We next turn to the computation of an upper bound of the RRF w.r.t. the considered uncertainty set, which is necessary for the proposed methods. For the chosen uncertainty set, an upper bound $\bar{u}$ of the RRF for (P) is given by

$$\bar{u} = \min_{j \in K} \frac{\max\{0, \bar{b}_j, \max\{|\bar{a}_i^j| : i = 1, ..., n\}\}}{\mu^j},$$

whereby K is the index set of the unsafe constraints. The value $\bar{u}$ is an upper bound for the RRF due to the following short explanation. If we assume that the RRF α satisfies $\alpha > \bar{u}$, then an index $k \in K$ exists such that $\pm\bar{a}_i^k \in \alpha\, \bar{\mathcal{U}}_{k_i}$ for $i \in \{1, ..., n\}$ and $-(\max\{0, \bar{b}^k\} + \varepsilon) \in \alpha\, \bar{\mathcal{U}}_{k_{\bar{b}}}$ for a sufficient small $\varepsilon > 0$ holds. Consequently, for every solution x a realization $u \in \bar{\mathcal{U}}_k$ exists such that

$$(\bar{a}^k)^T x + \alpha((u_I)^T x - u_{\bar{b}}) - \bar{b}^k > 0$$

holds, which directly implies the infeasibility of (EPR_α).

We now turn to the presentation and discussion of the numerical results. We note that we excluded the bounded IP approach in this numerical analysis because preliminary results showed that its performance is massively worse when compared to the other proposed methods. The performance of the proposed methods might differ between instances with positive RRF and instances with RRF zero. For example, if the RRF is zero, then only PureScaling automatically terminates after a single iteration independent from the chosen MIP gap. Consequently, we will separately analyze the numerical results for instances with positive RRF and with RRF zero. According to our results, the considered 165 instances split into the following sets: 66 instances with positive RRF, 85 instances with RRF zero, 13 instances which could not be solved in the timelimit of 2 h by any method, and one instance (`rmatr100-p10`) which could not be solved due to numerical issues. We now use log-scaled performance profiles to compare runtimes as proposed in [21]. We note that all runtimes include the computation of the upper bound. Figure 1 shows the performance profiles for instances with positive RRF and Figure 2 for instances with RRF zero. Furthermore, a short statistical summary of the runtimes and number of iterations is given in Tables 2 and 3. Overall, we see that the performance of the classical binary search and ScalingBin is nearly the same, independent from the RRF values. For instances with positive RRF, we see that the classical binary search, ScalingBin, and PureScaling solve the same number of instances, 97 % overall, while MaxScalingBin solves one instance less. In doing so, the best performance is given by PureScaling which outperforms the remaining methods. The performance of MaxScalingBin follows which is slightly better in comparison to the classic binary search, respectively ScalingBin. For instances with RRF zero, we recognize a similar performance pattern. This time the performances of MaxScalingBin and PureScaling are nearly identical and they outperform the other approaches in most of the cases. This improved performance of MaxScalingBin and PureScaling for instances with RRF zero is mainly explained by the fact that both algorithms almost always terminate after the first iteration, see Table 3. We note that this behavior is not necessarily guaranteed for MaxScalingBin in contrast to PureScaling due to the chosen MIP gap. However, the numerical results show that in most of the cases (SPRC_α) is solved to optimality in the first iteration, i.e., the corresponding objective value is zero. Consequently, a RRF of zero is immediately detected. MaxScalingBin as well as PureScaling solve 96 % of the instances with RRF zero, whereas the classic binary search and ScalingBin solve all of these instances. The effect that the latter two approaches solve slightly more instances can be explained by the fact that both methods only check feasibility in every iteration instead of solving the corresponding MIPs to optimality as in MaxScalingBin and PureScaling. Generally, the latter is more time-consuming.

Considering the number of iterations, maximizing the slack together with scaling the RRF, as proposed in MaxScalingBin and PureScaling, significantly reduces the

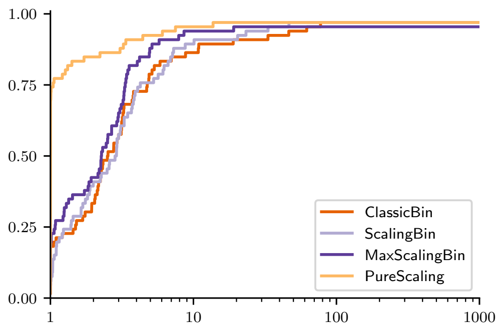

FIGURE 1. Log-scaled performance profiles of runtimes for instances with positive RRF

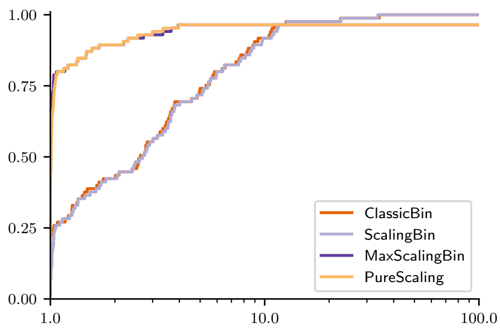

FIGURE 2. Log-scaled performance profiles of runtimes for instances with RRF zero

number of necessary iterations. In general, the number of iterations in MaxScalingBin is higher than in PureScaling because the latter checks in every iteration if the computed RRF is already in tolerance and does not have to lower an upper bound such as MaxScalingBin. Furthermore, it is interesting to see that scaling the RRF without maximizing the slack, as we do in ScalingBin, does not significantly decrease the necessary number of iterations, respectively the runtime, in comparison with the classical binary search. Furthermore, the statistical parameters of Tables 2 and 3 indicate that in most cases the RRF can be computed quickly ($< 60\,\mathrm{s}$). Only for a minority of the instances the runtimes drastically increase.

Based on the previous analysis of the results, we suggest to compute the RRF of a MIP as follows. First, run PureScaling with a small time or iteration limit. If the RRF could not be computed within the set limit, then we suggest to switch to the classical binary search, respectively to ScalingBin, because these methods solve more instances overall.

Finally, we turn to a short discussion about the price of robustness. To this end, we compare the optimal objective value of the nominal problem (P) and of the robust problem ($\mathrm{PR}_{\rho_{\mathrm{MIP}}}$). In the time limit of 2 h, we could optimally solve 51 of the 66 Problems ($\mathrm{PR}_{\rho_{\mathrm{MIP}}}$) with positive RRF. We then computed the price of robustness p as follows. Let the value w be the optimal nonzero objective value of (P) and w^* of ($\mathrm{PR}_{\rho_{\mathrm{MIP}}}$). Then, the price of robustness is given by $p = \frac{w^* - w}{|w|}$. As we can see in Table 4, the price of robustness is subject to strong fluctuations. On

Table 2. Number of solved instances (out of 66 instances with positive RRF) and statistics for the runtimes and number of iterations (always taken only for all instances solved to optimality)

	ClassicBin		ScalingBin		MaxScalingBin		PureScaling	
#solved	64		64		63		64	
	time/s	niter	time/s	niter	time/s	niter	time/s	niter
Minimum	0.23	15.00	0.13	1.00	0.11	1.00	0.11	1.00
1st Quartile	1.56	15.00	1.69	15.00	1.48	10.50	0.63	1.00
Median	7.30	15.00	9.20	15.00	6.85	14.00	3.35	1.00
Mean	315.12	17.50	259.72	16.13	196.18	13.38	251.98	3.22
3rd Quartile	82.98	18.00	83.27	17.00	42.59	17.00	42.67	3.00
Maximum	5800.64	32.00	6857.40	32.00	4276.22	32.00	4622.70	29.00

Table 3. Number of solved instances (out of 85 instances with RRF zero) and statistics for the runtimes and number of iterations (always taken only for all instances solved to optimality)

	ClassicBin		ScalingBin		MaxScalingBin		PureScaling	
#solved	85		85		82		82	
	time/s	niter	time/s	niter	time/s	niter	time/s	niter
Minimum	0.26	15.00	0.32	15.00	0.17	1.00	0.16	1.00
1st Quartile	5.69	15.00	5.95	15.00	2.14	1.00	2.15	1.00
Median	23.46	15.00	24.03	15.00	6.69	1.00	6.84	1.00
Mean	199.03	16.41	201.30	16.41	117.00	1.35	115.28	1.00
3rd Quartile	102.61	16.00	105.57	16.00	29.74	1.00	29.60	1.00
Maximum	4447.14	35.00	4490.15	35.00	2565.66	16.00	2567.18	1.00

the one hand instances with a small or even zero price of robustness exist. On the other hand for some instances the robustness of the solution comes along with an immense deterioration of the objective value. Surprisingly, the median shows that for many instances the price of robustness is in a reasonable limit keeping in mind that the considered uncertainty set has its maximal size w.r.t. robust feasibility. The results illustrate that choosing the "most robust" solution, as proposed in Section 1, does not necessarily come along with a high price of robustness. Furthermore, the price of robustness can be limited a priori by a so called budget constraint that is often desired in applications, see Section 1. Overall, the RRF can be useful as a decision rule to decide between different robust optimal solutions w.r.t. the size of the uncertainty set. We further note that the numerical results do not indicate relations between the percentage of unsafe constraints, the size of the RRF, and the price of robustness. The detailed numerical results of each instance can be found in our online supplement.

In practice, a decision maker often faces the following bi-objective challenge: On the one hand, one aims at guaranteeing robust feasibility of an optimal solution for the largest possible uncertainty set $\alpha\bar{\mathcal{U}}_j, j \in J$, i.e., one wants to maximize $\alpha \in [0, \rho_{\text{MIP}}]$, respectively $\alpha \in [0, \rho_{\text{MIP}}[$ if the RRF is not attained. On the other hand, however, one wants to minimize the optimal value of the robust counterpart or, equivalently, the price of robustness, which usually comes with a smaller α.

TABLE 4. Statistics for the best computed RRF and price of robustness (always taken only for all instances solved to optimality).

	Unsafe Constraints (%)	RRF	Price of Robustness (%)
Minimum	0.003	0.0001	0.00
1st Quartile	4.118	0.6200	93.28
Median	37.848	0.9901	384.16
Mean	43.015	67.0442	29 368 526 813.18
3rd Quartile	83.777	1.1509	20 877.96
Maximum	100.000	1006.0000	1 297 693 684 636.35

Consequently, a trade-off between robustness and minimum cost has to be made. We exemplarily illustrate three different characteristics for this trade-off in Figures 3-5, that we found in our computational experiments. To this end, we first discretized the interval $[0, \rho_{\mathrm{MIP}}]$ equidistantly and then computed the optimal value of the robust counterpart for each of these points. From Figure 3, it can be concluded that an increase in robustness comes with increasing cost, i.e., the price of robustness increases. Here, the trade-off between robustness and the optimal value is quite regular, i.e., for a possibly small increase of robustness, we always find a solution with a modest increase of cost. In contrast to this, we have a stepwise effect in Figure 4. Here, increasing the robustness can lead to two different effects regarding the cost. On the one hand, an increase of robustness can have almost no effect on the cost, which is for example the case for the interval $(0, 0.20)$. But on the other hand, pushing the robustness above a certain level, even by a really small increase, can lead to a very large increase of the cost, which is for example the case for a robustness level of at least 0.20. In Figure 5, both previously mentioned effects between robustness and cost exist. For $\alpha \in [0, 0.35]$, an increase of the robustness comes with larger cost, i.e., the price of robustness increases. In contrast to this, for $\alpha \in [0.35, 0.8509]$ an increase of the robustness comes with no or a modest increase of the optimal value of the robust counterpart.

Overall, an increase of robustness usually comes with an increase of the optimal value, i.e. the price of robustness increases. But as Figure 4 and 5 show, sometimes there is a possibility to significantly increase the robustness for small or no cost.

6. Conclusion

In this paper, we studied the problem of finding the "maximal" size of a given uncertainty set for a MIP such that its robust feasibility is guaranteed. In doing so, we determined this maximal size with the help of the radius of robust feasibility (RRF). We first motivated the investigations of this paper. We introduced the RRF for MIPs and then analyzed it w.r.t. its LP relaxation in the common setting of the literature. The latter requires a full-dimensional uncertainty set and thus, every variable is "unsafe". In particular, we proved that the RRF of a MIP and of its LP relaxation equal if the RRF of the relaxation is not attained. In special cases, this allows us to compute the RRF of a MIP with known techniques for the RRF of LPs. In order to make the RRF applicable to a broader spectrum of optimization problems, we extended the common setting of the RRF such that the uncertainty set is not necessarily full-dimensional and potentially different for every constraint. This allows to model safe variables and constraints, which are not affected by any uncertainty. We then proposed methods for computing the RRF of linear as well as mixed-integer problems in our extended setting. These methods can be seen as a first benchmark for computing the RRF including safe variables and constraints.

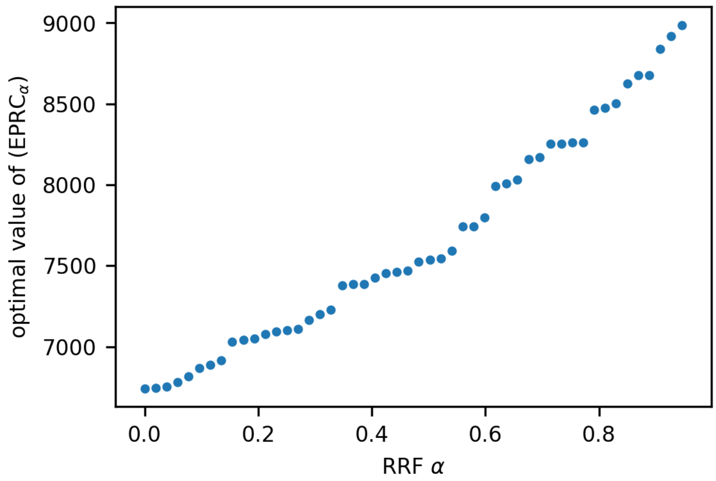

FIGURE 3. Trade-off between robustness and cost, i.e., optimal value of robust counterpart (EPRC$_\alpha$) as a function of the size of $\alpha\bar{\mathcal{U}}_j, j \in J$, for instance `binkar10_1` with RRF $\rho_{\text{MIP}} = 0.9459$.

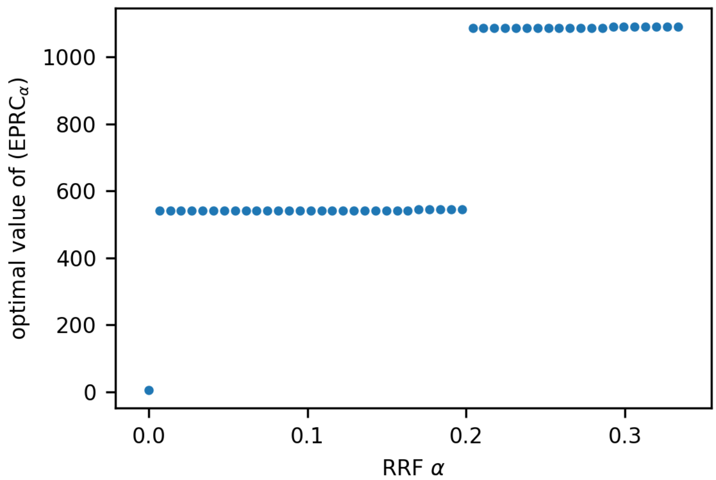

FIGURE 4. Trade-off between robustness and cost, i.e., optimal value of robust counterpart (EPRC$_\alpha$) as a function of the size of $\alpha\bar{\mathcal{U}}_j, j \in J$, for instance `comp07-2idx` with RRF $\rho_{\text{MIP}} = 0.3333$.

Finally, we illustrated the applicability of our methods by computing the RRF for MIPs of the MIPLIB 2017 library.

Further research and methods for computing the RRF in the extended framework are desirable, especially for a comparison with our methods. Also the extended RRF can now be applied to compute the "most robust" solution within an a priori budget for different applications. Additionally, it seems promising to use the information about the "maximal" size of an uncertainty set, computed by the RRF, in order to construct suitable uncertainty sets for robust optimization models. Moreover, sizing uncertainty sets w.r.t. alternative concepts of robustness, e.g., adjustable robustness, plays an important role in many applications: e.g., in gas networks

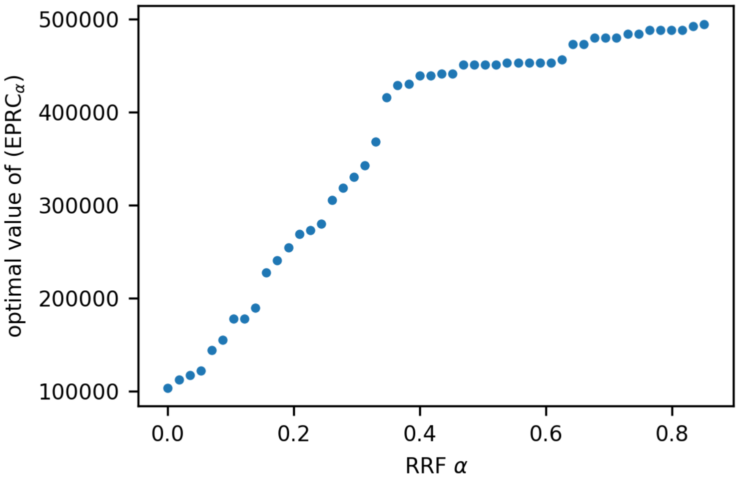

FIGURE 5. Trade-off between robustness and cost, i.e., optimal value of robust counterpart (EPRC$_\alpha$) as a function of size of $\alpha\bar{\mathcal{U}}_j, j \in J$, for instance `drayage-100-23` with RRF $\rho_{\text{MIP}} = 0.8509$.

it can be used for validating the feasibility of a booking [32] and for the optimal operation under technical uncertainties [1]. Thus, introducing the RRF for other concepts of robustness, especially adjustable robustness, are interesting topics for future research.

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Online Supplement
Radius of Robust Feasibility for Mixed-Integer Problems

Frauke Liers, Lars Schewe, Johannes Thürauf

Detailed Numerical Results

In this online supplement, we provide the detailed numerical results of our computational study. We list all instances for which we could not compute the RRF in our time limit of 2 h in Table 1. For instances with positive RRF, the best computed RRF, the percentage of unsafe constraints, and its price of robustness are given in Table 2. The detailed runtimes and number of iterations for instances with positive RRF are given in Table 3 and for instances with RRF zero in Table 4.

Table 1. Summary of instances that hit the timelimit of 2 h or could not be solved due to numerical issues (rmatr100-p10)

Instances	Unsafe Constraints (%)	RRF
cryptanalysiskb128n5obj16	44.950	–
glass4	90.909	–
neos-1456979	96.750	–
neos-2746589-doon	48.436	–
neos-3004026-krka	66.321	–
neos-3024952-loue	97.166	–
neos-3046615-murg	51.807	–
neos-3381206-awhea	99.165	–
neos-5107597-kakapo	98.938	–
nursesched-sprint02	0.568	–
rmatr100-p10	99.986	–
rmatr200-p5	99.997	–
supportcase26	95.402	–
swath3	42.986	–

TABLE 2. Summary price of robustness for instances with positive RRF (All values are standard rounded except of the RRF values. The latter values are rounded down in order to prevent an overestimation which can lead to an infeasibility of the corresponding robust counterpart. The computation of the price of robustness is based on the exact values of the numerical results)

Instances	Unsafe Constraints (%)	RRF	Nominal Objective	Robust Objective	Price of Robustness (%)
30n20b8	84.375	0.0156	302.00	604.00	100.00
50v-10	78.541	119.6930	3311.18	–	–
assign1-5-8	80.745	0.3846	212.00	–	–
binkar10_1	0.975	0.9459	6742.20	8986.79	33.29
bppc4-08	81.982	0.9999	53.00	–	–
brazil3	1.202	0.9999	24.00	–	–
buildingenergy	90.533	0.3975	33 283.85	782 078.32	2249.72
CMS750_4	66.821	0.0021	252.00	1000.00	296.83
comp07-2idx	0.513	0.3333	6.00	1091.00	18 083.30
cost266-UUE	3.942	0.5857	25 148 940.56	29 503 525.47	17.32
csched007	14.245	0.0296	351.00	590.40	68.20
csched008	14.245	0.9999	173.00	94 999 859.99	5.49×10^7
drayage-100-23	91.253	0.8509	103 333.87	494 653.66	378.70
drayage-25-23	91.253	0.8509	101 282.65	490 365.10	384.16
fiball	12.895	0.2790	138.00	1729.00	1152.90
gen-ip002	100.000	241.2800	−4783.73	−41.79	99.13
gen-ip054	100.000	1.1641	6840.97	7 231 278 446.60	1.06×10^8
gmu-35-40	3.774	0.1122	−2 406 733.37	−2 239 650.68	6.94
gmu-35-50	3.678	0.1122	−2 607 958.33	–	–
graphdraw-domain	39.306	0.1136	19 686.00	64 795.72	229.15
ic97_potential	91.013	0.0204	3942.00	4255.31	7.95
leo1	14.840	0.9333	404 227 536.16	–	–

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TABLE 2. Summary price of robustness for instances with positive RRF (All values are standard rounded except of the RRF values. The latter values are rounded down in order to prevent an overestimation which can lead to an infeasibility of the corresponding robust counterpart. The computation of the price of robustness is based on the exact values of the numerical results)

Instances	Unsafe Constraints (%)	RRF	Nominal Objective	Robust Objective	Price of Robustness (%)
leo2	24.789	0.9333	404 077 441.12	–	–
mad	21.569	16.3333	0.03	2.02	7437.31
mas74	92.308	0.9999	11 801.19	118 171 839.07	1.00×10^6
mas76	91.667	0.9999	40 005.05	837 260 542 319.45	2.09×10^9
mc11	79.167	0.9814	11 689.00	128 960.00	1003.26
mik-250-20-75-4	38.462	951.0000	−52 301.00	0.00	100.00
mushroom-best	99.953	0.9090	0.06	3916.90	7.08×10^6
n3div36	1.293	2.9897	130 800.00	–	–
n5-3	9.416	226.3543	8105.00	–	–
n9-3	7.107	218.5548	14 409.00	–	–
neos-1122047	100.000	0.0001	161.00	162.00	0.62
neos-3083819-nubu	0.127	907.2763	6 307 996.00	7 019 780.00	11.28
neos-4763324-toguru	49.676	0.9999	1613.04	–	–
neos-662469	37.235	0.3333	184 380.00	–	–
neos-787933	92.989	44.0000	30.00	1764.00	5780.00
neos-860300	60.000	6.6666	3201.00	3201.00	0.00
neos-911970	44.860	0.9999	54.76	232 510 087.68	4.25×10^8
neos-933966	26.920	0.9999	318.00	4 126 665 917 461.59	1.30×10^{12}
neos17	99.794	416.9255	0.15	1.62	979.91
neos5	95.238	0.7272	15.00	60.00	300.00
nexp-150-20-8-5	50.455	0.9749	231.00	–	–
ns1760995	0.032	0.7225	−549.21	−69.06	87.43

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TABLE 2. Summary price of robustness for instances with positive RRF (All values are standard rounded except of the RRF values. The latter values are rounded down in order to prevent an overestimation which can lead to an infeasibility of the corresponding robust counterpart. The computation of the price of robustness is based on the exact values of the numerical results)

Instances	Unsafe Constraints (%)	RRF	Nominal Objective	Robust Objective	Price of Robustness (%)
nu25-pr12	5.015	0.9999	53 905.00	212 500 011 900.00	3.94×10^8
p200x1188c	85.591	1.9969	15 078.00	3 584 430.00	23 672.60
pg	20.000	1006.0000	−8674.34	7018.05	180.91
pk1	66.667	0.9999	11.00	7 641 184.01	6.95×10^7
rail02	0.003	1.0000	−200.45	−199.86	0.29
ran14x18-disj-8	81.655	0.8666	3712.00	42 404.10	1042.35
reblock115	0.422	219.5121	−36 800 603.23	0.00	100.00
rococoB10-011000	5.399	0.8959	19 449.00	108 960.00	460.23
rococoC11-011100	4.647	0.9029	20 889.00	146 524.00	601.44
s250r10	0.146	1.1111	−0.17	–	–
satellites2-40	13.731	0.0001	−19.00	−16.00	15.79
satellites2-60-fs	17.389	0.0001	−19.00	−16.00	15.79
savsched1	0.886	0.9999	3217.70	3 858 535 013.84	1.20×10^8
seymour1	86.064	0.3333	410.76	587.59	43.05
sp150x300d	66.667	5.1388	69.00	300.00	334.78
square41	0.090	0.9988	15.00	1681.00	11 106.70
square47	0.068	0.9990	16.00	2209.00	13 706.30
supportcase18	50.000	0.8666	48.00	120.00	150.00
supportcase42	100.000	0.9999	7.76	15 271 400 016.50	1.97×10^{11}
swath1	42.986	0.7576	379.07	–	–
trento1	1.265	0.8552	5 189 487.00	9 993 978 424.72	192 481
var-smallemery-m6j6	1.118	6.8910	−149.38	226.79	251.83

TABLE 3. Runtimes and number of iterations for instances with positive RRF (all values are standard rounded)

Instances	ClassicBin		ScalingBin		maxScalingBin		PureScaling	
	time/s	niter	time/s	niter	time/s	niter	time/s	niter
`30n20b8`	**13.62**	15	14.11	15	42.58	13	60.24	**6**
`50v-10`	1.56	16	1.70	16	0.70	10	**0.49**	**2**
`assign1-5-8`	80.56	17	80.81	17	13.69	17	**1.74**	**2**
`binkar10_1`	1.98	18	2.76	16	3.02	17	**0.92**	**3**
`bppc4-08`	3.92	20	4.87	20	3.86	20	**0.67**	**1**
`brazil3`	227.63	15	227.89	15	**6.85**	**1**	6.89	**1**
`buildingenergy`	**1903.99**	**15**	1975.59	**15**	$>$ 7200	–	$>$ 7200	–
`CMS750_4`	9.10	15	10.10	15	8.84	13	**3.93**	**2**
`comp07-2idx`	7.01	15	6.57	12	4.03	14	**4.01**	**2**
`cost266-UUE`	6.01	32	6.32	32	13.88	32	**1.62**	**1**
`csched007`	**346.43**	16	346.56	16	$>$ 7200	–	2593.44	4
`csched008`	1.25	15	1.26	15	0.39	**1**	**0.38**	**1**
`drayage-100-23`	7.07	30	9.24	29	7.76	29	**3.16**	**3**
`drayage-25-23`	7.03	30	9.16	29	8.12	29	**3.24**	**3**
`fiball`	**23.28**	15	26.82	14	40.24	11	51.70	**10**
`gen-ip002`	0.25	15	0.13	2	**0.12**	**1**	0.13	**1**
`gen-ip054`	0.37	15	0.36	15	**0.22**	**11**	0.67	29
`gmu-35-40`	2449.44	15	13.61	15	13.51	14	**7.26**	**4**
`gmu-35-50`	3893.63	15	1464.00	15	**62.83**	11	211.56	**7**
`graphdraw-domain`	2052.99	15	2049.67	15	4276.22	11	**1695.64**	**5**
`ic97_potential`	90.23	21	90.63	21	43.12	18	**39.95**	**9**
`leo1`	26.07	15	35.58	14	15.57	12	**5.35**	**2**
`leo2`	97.17	15	121.69	14	41.17	12	**13.89**	**2**

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TABLE 3. Runtimes and number of iterations for instances with positive RRF (all values are standard rounded)

Instances	ClassicBin		ScalingBin		maxScalingBin		PureScaling	
	time/s	niter	time/s	niter	time/s	niter	time/s	niter
`mad`	0.26	15	0.26	14	**0.25**	14	0.42	**4**
`mas74`	0.58	28	0.66	28	0.60	28	**0.18**	**1**
`mas76`	0.53	28	0.68	28	0.59	28	**0.18**	**1**
`mc11`	1.96	23	2.31	23	2.12	23	**0.63**	**1**
`mik-250-20-75-4`	1.24	16	1.20	15	1.40	16	**0.64**	**3**
`mushroom-best`	40.92	15	54.92	15	25.36	11	**7.68**	**1**
`n3div36`	463.74	15	432.79	15	55.37	8	**42.86**	**3**
`n5-3`	1.34	15	1.50	15	1.64	13	**1.22**	**3**
`n9-3`	4.18	15	4.90	15	**2.79**	13	3.54	**2**
`neos-1122047`	35.61	15	38.03	15	46.73	15	**15.27**	**1**
`neos-3083819-nubu`	1.59	15	0.58	2	**0.42**	**1**	0.44	**1**
`neos-4763324-toguru`	**131.56**	23	145.39	23	298.17	22	798.40	**2**
`neos-662469`	65.61	15	70.40	14	17.10	14	**3.46**	**1**
`neos-787933`	70.45	16	69.52	16	60.03	16	**22.40**	**1**
`neos-860300`	42.63	15	43.74	14	42.61	14	**8.30**	**1**
`neos-911970`	0.89	17	1.05	17	0.96	17	**0.28**	**1**
`neos-933966`	9.60	15	14.28	15	5.00	**1**	**4.93**	**1**
`neos17`	2.00	16	2.39	16	2.54	15	**1.32**	**6**
`neos5`	0.47	15	0.61	15	0.40	13	**0.19**	**1**
`nexp-150-20-8-5`	**22.55**	15	24.78	15	28.09	**12**	73.01	21
`ns1760995`	878.32	15	878.51	15	762.52	12	**609.89**	**4**
`nu25-pr12`	2.93	15	3.67	15	**0.60**	**1**	**0.60**	**1**
`p200x1188c`	1.55	26	1.67	26	1.72	26	**0.41**	**1**

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TABLE 3. Runtimes and number of iterations for instances with positive RRF (all values are standard rounded)

Instances	ClassicBin		ScalingBin		maxScalingBin		PureScaling	
	time/s	niter	time/s	niter	time/s	niter	time/s	niter
`pg`	1.04	15	**0.22**	**1**	0.24	**1**	0.27	**1**
`pk1`	0.23	15	0.16	15	**0.11**	**1**	**0.11**	**1**
`rail02`	$>$ 7200	–	$>$ 7200	–	$>$ 7200	–	**4280.51**	**1**
`ran14x18-disj-8`	**1.27**	15	2.14	15	1.56	14	1.80	**9**
`reblock115`	0.96	15	0.36	2	0.37	**1**	**0.35**	**1**
`rococoB10-011000`	7.53	22	3.92	21	2.25	22	**0.69**	**1**
`rococoC11-011100`	3.25	22	3.18	22	3.32	22	**1.03**	**1**
`s250r10`	217.94	15	171.28	3	**24.75**	**1**	24.96	**1**
`satellites2-40`	6.26	15	6.58	15	6.83	15	**2.95**	**1**
`satellites2-60-fs`	4.53	15	4.77	15	4.39	15	**1.64**	**1**
`savsched1`	124.35	15	180.82	15	**42.52**	**1**	42.60	**1**
`seymour1`	6.81	15	9.01	15	5.86	14	**1.45**	**1**
`sp150x300d`	0.44	24	0.51	24	0.40	24	**0.18**	**1**
`square41`	5800.64	15	6857.40	8	266.05	5	**74.89**	**1**
`square47`	$>$ 7200	–	$>$ 7200	–	743.13	5	**248.40**	**1**
`supportcase18`	**17.49**	18	18.61	17	334.40	15	239.92	**2**
`supportcase42`	**57.63**	15	114.86	15	105.69	**2**	76.04	**2**
`swath1`	**73.76**	19	74.16	19	2671.01	19	4622.70	**10**
`trento1`	**350.85**	**16**	354.43	**16**	1724.57	**16**	$>$ 7200	–
`var-smallemery-m6j6`	461.69	21	526.71	21	457.99	20	**203.29**	**7**

TABLE 4. Runtimes and number of iterations for instances with RRF zero (all values are standard rounded)

Instances	ClassicBin		ScalingBin		maxScalingBin		PureScaling	
	time/s	niter	time/s	niter	time/s	niter	time/s	niter
academictimetablesmall	69.20	16	69.23	16	67.34	**1**	**67.26**	**1**
app1-2	25.48	15	25.78	15	**20.14**	**1**	20.37	**1**
atlanta-ip	59.33	15	61.03	15	**8.07**	**1**	8.13	**1**
beasleyC3	1.06	21	1.06	21	**0.28**	**1**	0.30	**1**
bnatt400	564.01	16	564.76	16	158.92	**1**	**158.79**	**1**
cbs-cta	5.67	15	5.95	15	**1.15**	**1**	1.16	**1**
cmflsp50-24-8-8	73.25	15	73.38	15	**23.22**	**1**	23.25	**1**
co-100	211.70	15	215.46	15	**25.26**	**1**	26.20	**1**
dano3_3	**20.21**	15	20.58	15	79.85	**1**	80.25	**1**
dano3_5	**20.87**	15	21.03	15	161.70	**1**	162.33	**1**
decomp2	5.33	16	5.37	16	1.93	**1**	**1.91**	**1**
exp-1-500-5-5	0.40	24	0.38	24	0.17	**1**	**0.16**	**1**
fastxgemm-n2r6s0t2	3.83	15	3.96	15	**3.04**	**1**	3.05	**1**
germanrr	220.16	16	220.30	16	5.58	**1**	**5.49**	**1**
h80x6320d	5.30	23	5.06	23	**0.93**	**1**	0.98	**1**
hypothyroid-k1	**70.67**	16	73.34	16	94.91	**1**	94.67	**1**
irish-electricity	87.55	15	88.96	15	36.56	**1**	**36.32**	**1**
istanbul-no-cutoff	13.25	15	13.62	15	**4.68**	**1**	4.74	**1**
k1mushroom	**381.57**	19	396.44	19	504.87	**1**	505.16	**1**
lectsched-5-obj	70.85	15	71.73	15	**6.66**	**1**	6.77	**1**
lotsize	11.90	29	11.72	29	**0.35**	**1**	0.37	**1**
map10	332.48	15	335.44	15	**249.34**	**1**	250.87	**1**
map16715-04	336.61	15	337.06	15	250.81	**1**	**250.11**	**1**

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TABLE 4. Runtimes and number of iterations for instances with RRF zero (all values are standard rounded)

Instances	ClassicBin		ScalingBin		maxScalingBin		PureScaling	
	time/s	niter	time/s	niter	time/s	niter	time/s	niter
`mcsched`	0.26	15	0.32	15	**0.18**	**1**	0.19	**1**
`milo-v12-6-r2-40-1`	9.62	20	9.64	20	**2.65**	**1**	2.66	**1**
`momentum1`	92.91	15	93.54	15	**4.11**	**1**	4.25	**1**
`mzzv11`	1.62	15	1.57	15	1.43	**1**	**1.38**	**1**
`mzzv42z`	3.95	15	3.80	15	1.55	**1**	**1.53**	**1**
`n2seq36q`	1063.70	**16**	**1062.89**	**16**	>7200	–	>7200	–
`neos-1171448`	16.10	16	16.94	16	**2.08**	**1**	2.12	**1**
`neos-1171737`	8.33	17	8.66	17	**0.89**	**1**	0.92	**1**
`neos-1354092`	4447.14	15	4490.15	15	**504.62**	**1**	504.71	**1**
`neos-1582420`	**5.55**	15	5.60	15	20.31	15	16.59	**1**
`neos-2657525-crna`	1.43	17	1.47	17	**1.33**	**1**	1.33	**1**
`neos-2978193-inde`	**4.72**	18	4.80	18	5.50	**1**	5.44	**1**
`neos-3216931-puriri`	96.38	16	96.38	16	**17.27**	**1**	17.33	**1**
`neos-3627168-kasai`	1.20	27	1.21	27	**0.44**	**1**	0.45	**1**
`neos-4413714-turia`	83.27	16	89.39	16	15.44	**1**	**15.05**	**1**
`neos-4532248-waihi`	**817.56**	16	819.32	16	2224.22	16	2090.09	**1**
`neos-4722843-widden`	21.60	15	21.71	15	15.54	**1**	**14.99**	**1**
`neos-4738912-atrato`	3.41	18	3.32	18	**0.52**	**1**	0.54	**1**
`neos-5049753-cuanza`	**437.25**	15	444.66	15	529.72	**1**	529.12	**1**
`neos-5075914-elvire`	2526.50	**15**	**2526.25**	**15**	>7200	–	>7200	–
`neos-5188808-nattai`	23.46	15	24.03	15	**6.51**	**1**	**6.51**	**1**
`neos-5195221-niemur`	17.78	15	18.32	15	**11.96**	**1**	12.09	**1**
`neos-631710`	**46.16**	**17**	47.00	**17**	>7200	–	>7200	–

Continued on next page

TABLE 4. Runtimes and number of iterations for instances with RRF zero (all values are standard rounded)

Instances	ClassicBin		ScalingBin		maxScalingBin		PureScaling	
	time/s	niter	time/s	niter	time/s	niter	time/s	niter
neos-827175	**12.02**	15	12.46	15	20.32	**1**	20.27	**1**
neos-848589	270.69	35	277.71	35	**153.31**	**1**	153.33	**1**
neos-873061	378.84	15	380.52	15	226.97	**1**	**224.59**	**1**
neos-950242	9.93	15	9.85	15	**6.04**	**1**	**6.04**	**1**
neos-957323	18.75	15	19.15	15	**6.73**	**1**	6.91	**1**
neos-960392	**5.69**	15	5.76	15	19.06	**1**	19.09	**1**
neos8	23.48	15	24.16	15	9.39	**1**	**9.27**	**1**
net12	14.07	15	14.41	15	2.30	**1**	**2.22**	**1**
ns1116954	**1113.99**	15	1122.95	15	2565.66	**1**	2567.18	**1**
ns1208400	16.32	15	16.48	15	**16.11**	**1**	**16.11**	**1**
ns1644855	247.80	15	262.14	15	23.03	**1**	**22.90**	**1**
ns1830653	14.35	16	14.58	16	**1.89**	**1**	1.92	**1**
peg-solitaire-a3	157.90	16	**157.72**	16	246.30	**1**	246.12	**1**
pg5_34	1.82	20	1.84	20	**1.75**	**1**	1.76	**1**
physiciansched3-3	353.65	15	359.83	15	177.99	**1**	**175.61**	**1**
physiciansched6-2	76.86	15	77.16	15	**61.08**	**1**	61.61	**1**
piperout-08	6.13	15	6.21	15	**5.05**	**1**	5.13	**1**
radiationm18-12-05	15.95	15	16.29	15	4.48	**1**	**4.31**	**1**
rail01	**461.10**	16	461.55	16	679.00	**1**	678.23	**1**
rd-rplusc-21	461.78	15	483.85	15	134.18	**1**	**132.79**	**1**
rocI-4-11	4.18	15	4.18	15	1.40	**1**	**1.39**	**1**
rocII-5-11	82.81	15	83.64	15	**6.58**	**1**	6.60	**1**
roi2alpha3n4	113.86	17	118.77	17	**10.26**	**1**	10.41	**1**

Continued on next page

TABLE 4. Runtimes and number of iterations for instances with RRF zero (all values are standard rounded)

Instances	ClassicBin		ScalingBin		maxScalingBin		PureScaling	
	time/s	niter	time/s	niter	time/s	niter	time/s	niter
`roll3000`	3.28	15	3.26	15	0.70	**1**	**0.68**	**1**
`sct2`	2.48	15	2.54	15	**0.50**	**1**	**0.50**	**1**
`snp-02-004-104`	13.46	15	13.77	15	**5.12**	**1**	5.18	**1**
`sp97ar`	32.29	15	33.98	15	**3.91**	**1**	4.00	**1**
`sp98ar`	47.00	15	51.23	15	**5.24**	**1**	5.29	**1**
`supportcase12`	102.61	15	105.57	15	29.87	**1**	**29.85**	**1**
`supportcase33`	18.95	15	19.27	15	**3.56**	**1**	3.73	**1**
`supportcase40`	17.96	15	19.10	15	**5.53**	**1**	5.62	**1**
`supportcase7`	302.96	15	318.74	15	29.36	**1**	**28.86**	**1**
`tr12-30`	**0.64**	25	0.68	25	0.94	**1**	0.94	**1**
`traininstance6`	3.22	15	3.22	15	**0.96**	**1**	1.01	**1**
`triptim1`	41.73	15	41.52	15	**19.92**	**1**	**19.92**	**1**
`uccase12`	71.50	15	75.47	15	**18.79**	**1**	18.97	**1**
`uccase9`	45.94	15	46.08	15	10.10	**1**	**10.07**	**1**
`uct-subprob`	**1.53**	15	1.59	15	3.37	**1**	3.35	**1**
`unitcal_7`	29.77	15	30.48	15	**5.11**	**1**	5.13	**1**

Article 2

Structural properties of feasible bookings in the European entry-exit gas market system

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Structural Properties of Feasible Bookings in the European Entry-Exit Gas Market System

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Abstract. In this work, we analyze the structural properties of the set of feasible bookings in the European entry-exit gas market system. We present formal definitions of feasible bookings and then analyze properties that are important if one wants to optimize over them. Thus, we study whether the sets of feasible nominations and bookings are bounded, convex, connected, conic, and star-shaped. The results depend on the specific model of gas flow in a network. Here, we discuss a simple linear flow model with arc capacities as well as nonlinear and mixed-integer nonlinear models of passive and active networks, respectively. It turns out that the set of feasible bookings has some unintuitive properties. For instance, we show that the set is nonconvex even though only a simple linear flow model is used.

1. Introduction

Mathematical optimization of gas transport networks has been a highly active field of research during the last decades. For an overview of the field see, e.g., the recent book [35] and the recent survey article [44] as well as the references therein. Most of the research in this field so far dealt with the case of a single pattern of supplies and withdrawals (which we will call a nomination throughout the paper) that need to be transported through a given network. In this setting, two major tasks for mathematical optimization arise:

Feasibility: Given a nomination, check whether it is feasible w.r.t. physical and technical laws and rules.

Optimization: Given a feasible nomination, determine the cheapest way of transporting the nomination.

Both questions have been addressed very comprehensively in the literature of the last 50 years; see, e.g., [2–5, 10, 11, 15, 22, 23, 29–31, 37–39, 41, 43, 47, 54] to name only a few publications that stem from different fields of mathematical optimization like mixed-integer linear optimization, nonlinear optimization, robust optimization, optimization with complementarity constraints, or optimization with partial differential equations.

However, since the gas market liberalization that started in the 1990s, also other mathematical questions came up. In Europe, the gas market liberalization lead to the entry-exit system; see, e.g., [13, 17, 18]. At the core of this system, the interplay of so-called bookings and nominations has been established. A booking is a mid- to long-term contract between a gas trader and a gas transport company in which a capacity right is granted to the trader. This means, that for a booking $b \geq 0$, the trader has the right to nominate (for the day ahead) every amount below, i.e., every amount ℓ with $0 \leq \ell \leq b$, if it is in balance with all other nominations. By signing such a booking contract, the gas transport company guarantees that every

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balanced set of nominations that is in compliance with the corresponding bookings can actually be transported.

In contrast to the rich literature on nominations, there is much less literature on the mathematics of bookings. Among the first mathematical treatments of bookings are the two PhD theses [32, 53] and the technical report [20]. Moreover, a rather detailed discussion is given in Part III of the book [35]. From a mathematical point of view, the feasibility of a booking can be seen as some special case of robust feasibility in the sense of robust optimization [6]. In this context, an efficient test for checking the feasibility of a booking in a passive tree-structured network is given in [45] and the feasibility of bookings as well as complexity results for checking this feasibility is studied in [36]. Other related problems like the computation of maximum possible bookings (the so-called technical capacity) are introduced in [40]. Lastly, we also want to mention studies like they can be found in [1, 7], where entry-exit tariffs are discussed but where the authors do not study feasibility or optimization questions based on bookings.

Since the concept of bookings is at the interface of gas transport and trading, it needs to be studied both from a technical and physical as well as from an economic viewpoint. The latter is, e.g., given in [27], where a mathematical multilevel model of the European entry-exit system is presented that also includes the trading of booking contracts. Other modeling approaches for economic questions in gas markets have been discussed recently in [26]. In mathematical economics, the general hardness of multilevel or equilibrium models often requires to abstract from certain physical details of gas flow models. This is why linear flow models are often discussed in this area; see, e.g., [8, 9, 12, 14, 21, 42, 52] and the references therein. As a consequence, the consideration of bookings also needs to be done on different levels of physical and technical modeling of gas transport networks—ranging from very simple linear models to highly sophisticated nonlinear ones [50].

The above discussion is the main motivation for this paper. We analyze structural properties of the set of feasible nominations and bookings. As already discussed above, the structural properties of the set of feasible nominations has already been discussed in the literature. Thus, we focus on the set of feasible bookings. Moreover, and in contrast to the existing literature, we do not consider the set of feasible nominations structurally "only" for the case in passive but also in gas transport networks that include active elements such as compressors. The analysis of the set of feasible bookings and nominations is an important prerequisite for deciding feasibility of bookings or for optimizing over these sets. Our contribution is the following. We formalize the concept of bookings and study the set of feasible nominations and bookings for three important and different classes of gas flow models:

(a) a linear flow model with arc capacities;
(b) a nonlinear flow model for passive networks, i.e., for networks without controllable elements like compressors or valves;
(c) a nonlinear flow model for active networks, i.e., for networks with controllable elements.

For these models, we prove or present counterexamples for the boundedness, convexity, and connectivity of the set of feasible nominations and bookings and additionally study whether it is conic or star-shaped. By this, we pave the way for further studies like, e.g., computing the largest possible bookings, which is of practical importance for gas transport companies. Our results show that one needs to be very careful when considering bookings because rather unintuitive properties can be observed—for instance that we obtain a nonconvex set of feasible bookings even for linear flow models. This is mainly based on the definition of a feasible booking b, which requires that *every* balanced and component-wise smaller nomination

$0 \leq \ell \leq b$ is feasible. At this point, let us note that the rather counter-intuitive definition considered in this paper is chosen as it is discussed in the respective legislative texts on the European entry-exit gas market system; see [17, 18]. The motivation of the notion of bookings in particular and the European entry-exit system in general is the decoupling of economic trading and the technical transport through the network. Since a feasible booking guarantees the feasibility of every balanced and component-wise smaller nomination, no further technical restrictions for trading booking-compliant nominations exist. Thus, economic trading and the technical transport of gas are decoupled.

We remark that all models studied in this paper describe stationary flows. Since unexpected effects w.r.t. bookings already appear in these simplified gas transport models, it is likely to assume that this is also the case in more detailed gas transport models—most probably, it will even be more pronounced. The analysis of transient flow models as well as even more complicated stationary flow models is out of scope of this paper and part of our future research.

The remainder of the paper is structured as follows. In Section 2 we introduce the basic definitions and discuss a preliminary example of a very basic gas flow model in order to illustrate the concepts that we afterward analyze for more complicated models. The Sections 3–5 then analyze the properties of the set of feasible bookings for a linear flow model with arc capacities (Section 3), a nonlinear flow model (Section 4), and a mixed-integer nonlinear flow model (Section 5) in which controllable elements are modeled using binary variables. Finally, we conclude in Section 6 and pose some questions for future research.

2. Basic Definitions

We model a gas network as a directed graph $G = (V, A)$ with node set V and arc set A. The set of nodes is partitioned into the set V_+ of entry nodes, at which gas is supplied, the set V_- of exit nodes, where gas is withdrawn, and the set V_0 of the remaining inner nodes. We abbreviate the set $V_+ \cup V_-$ by V_b. The orientation of the arcs is artificial and thus negative flow along an arc can occur. In real-world gas networks, the arc set is typically partitioned into different types of arcs that correspond to different elements of the network; e.g., pipes, compressors, etc. We introduce these sets when we consider them for the first time. Finally, we always assume in the following that the undirected graph underlying G is connected. We now introduce basic definitions that we use in the following.

Definition 2.1 (Load flow)**.** A *load flow* is a vector

$$\ell = (\ell_u)_{u \in V_\mathrm{b}} \in \mathbb{R}^{V_\mathrm{b}}_{\geq 0}.$$

The set of load flow vectors is denoted by L.

A load flow thus corresponds to an actual situation at a single point in time by specifying the amount of gas that is supplied (ℓ_u for $u \in V_+$) or withdrawn (ℓ_u for $u \in V_-$). Since we only consider stationary flows, we need to impose that the supplied amount of gas equals the withdrawn amount, which leads to the definition of a nomination.

Definition 2.2 (Nomination)**.** A *nomination* is a balanced load flow ℓ, i.e., $\sigma^\top \ell = 0$ with $\sigma \in \{\pm 1\}^{V_\mathrm{b}}, \sigma_u = 1$ for all $u \in V_+$, $\sigma_u = -1$ for all $u \in V_-$. The set of nominations is called N, i.e.,

$$N := \{\ell \in L : \sigma^\top \ell = 0\} \subseteq L.$$

Definition 2.3 (Booking)**.** A *booking* is a vector $b = (b_u)_{u \in V_\mathrm{b}} \in \mathbb{R}^{V_\mathrm{b}}_{\geq 0}$. The set of bookings is denoted by B.

Nominations and bookings are connected by the following definition.

Definition 2.4 (Booking-compliant nomination)**.** A nomination ℓ is called *booking-compliant* with respect to the booking b if $\ell \leq b$ holds, where "$\leq$" is meant component-wise. The set of booking-compliant (or b-compliant) nominations is given by

$$N(b) := \{\ell \in N : \ell \leq b\}.$$

Obviously, $N(b) \subseteq N \subseteq L$ holds for finite b.

We now define *feasible nominations* and *feasible bookings*, where "feasible" is meant with respect to technical, physical, and legal constraints of gas transport. To this end, let $c_{\mathcal{E}}(x, s; \ell) = 0$ and $c_{\mathcal{I}}(x, s; \ell) \geq 0$ be the possibly nonlinear, nonconvex, and nonsmooth constraints that model the full problem of gas transport possibly including models of nodes, pipes, compressors, etc. Moreover, let $z := (x, s) \in \mathbb{R}^{n_x} \times \mathbb{Z}^{n_s}$ be the discrete-continuous variable vector that is required to state this model.

Definition 2.5 (Feasible nomination)**.** A nomination $\ell \in N$ is *feasible* if a vector $z := (x, s) \in \mathbb{R}^{n_x} \times \mathbb{Z}^{n_s}$ exists such that

$$c_{\mathcal{E}}(x, s; \ell) = 0, \quad c_{\mathcal{I}}(x, s; \ell) \geq 0 \tag{1}$$

holds. The set of feasible nominations is denoted by F_N.

We note that the set of feasible nominations F_N depends on the chosen model of gas transport. The only constraint that we need in all formulations is mass conservation at each node of the network that is modeled by Kirchhoff's first law, i.e.,

$$\sum_{a \in \delta^{\text{out}}(u)} q_a - \sum_{a \in \delta^{\text{in}}(u)} q_a = q_u \quad \text{for all } u \in V, \tag{2}$$

where $q_u \geq 0$ for entries, $q_u \leq 0$ for exits, and $q_u = 0$ for inner nodes.

The dependency of the feasible set defined by (1) on the nomination is given by fixing the entry and exit flows according to the nomination ℓ, i.e.,

$$q_u = \ell_u \quad \text{for all } u \in V_+, \quad q_u = -\ell_u \quad \text{for all } u \in V_-.$$

These constraints are part of $c_{\mathcal{E}}(x, s; \ell) = 0$ in (1).

We note that to check whether a given nomination is feasible may lead to a mixed-integer nonlinear and nonconvex problem depending on the constraints $c_{\mathcal{E}}$ and $c_{\mathcal{I}}$. For more information on this problem, see [35] or [43] and the references therein.

Definition 2.6 (Feasible booking)**.** We say that a booking b is *feasible* if all booking-compliant nominations $\ell \in N(b)$ are feasible. The set of feasible bookings is denoted by F_B.

The definition of a feasible booking is very strict and may appear counter-intuitive at a first glance. However, this definition directly follows from the legislative texts about the European entry-exit gas market system, which aims at decoupling the economic trading and the technical transport of the gas.

For later reference, we also state definitions of cones and star-shaped sets; see [33] for more details.

Definition 2.7 (Cone)**.** The set $K \subseteq \mathbb{R}^n$ is a *cone*, if $\lambda x \in K$ holds for any $x \in K$ and $\lambda \geq 0$.

Definition 2.8 (Star-shaped set)**.** The set $K \subseteq \mathbb{R}^n$ is *star-shaped* w.r.t. $x_0 \in K$ if for every element $x \in K$ and $\lambda \in [0, 1]$ the relation

$$\lambda x + (1 - \lambda)x_0 \in K$$

holds.

TABLE 1. Properties of F_N and F_B w.r.t. the simple gas transport model (3)

Properties	Gas transport constraints (3)
Bounded F_N	×
Bounded F_B	×
Convex F_N	✓
Convex F_B	✓
Connected F_N	✓
Connected F_B	✓
Star-shaped F_N	✓
Star-shaped F_B	✓
Conic F_N	✓
Conic F_B	✓

From the definition of a star-shaped set K w.r.t. x_0 it directly follows that for each element $x \in K$ the line segment $[x_0, x]$ is contained in K.

In the remainder of this paper, we always consider the point of view of a transmission system operator (TSO) and we thus focus on technical and physical restrictions of the gas network. As a preliminary example let us first consider the case that except of Kirchhoff's first law (2) no further restrictions for gas transport exist. Hence, for a nomination $\ell \in N$ the Constraints (1) are given by

$$\sum_{a \in \delta^{\text{out}}(u)} q_a - \sum_{a \in \delta^{\text{in}}(u)} q_a = \sigma_u \ell_u \quad \text{for all } u \in V, \tag{3}$$

i.e.,

$$c_{\mathcal{E}}(x, s; \ell) = c_{\mathcal{E}}(x; \ell) = (c_{\mathcal{E},u}(q; \ell))_{u \in V}$$

with

$$c_{\mathcal{E},u}(q; \ell) = \sum_{a \in \delta^{\text{out}}(u)} q_a - \sum_{a \in \delta^{\text{in}}(u)} q_a - \sigma_u \ell_u$$

and $c_{\mathcal{I}}(x, s; \ell)$ is empty. Moreover, we set $\ell_u = \sigma_u = 0$ for all inner nodes $u \in V_0$ in Constraint (3).

We now analyze the feasibility of nominations and bookings w.r.t. (3). Each nomination ℓ of the set of nominations N is feasible, which can be shown by a direct proof or by Theorem 7.1 in [34]. The feasibility of each nomination implies that the set of feasible nominations F_N is unbounded, convex, connected, conic, and star-shaped. Furthermore, it follows that each booking is feasible and that the set of feasible bookings F_B has the same properties as the set of feasible nominations. We summarized the results w.r.t. linear flow without arc capacities in Table 1.

3. A Capacitated Linear Flow Model

In addition to the model used in the last section, we now further assume lower and upper flow bounds $q_a^- \le q_a^+$ to be given for every arc $a \in A$. That means, we consider a standard capacitated linear flow model. Consequently, for a nomination $\ell \in N$ the Constraints (1) are given by (3) and the flow bounds

$$q_a^- \le q_a \le q_a^+ \quad \text{for all } a \in A, \tag{4}$$

i.e.,

$$c_{\mathcal{I}}(x, s; \ell) = c_{\mathcal{I}}(x; \ell) = (c_{\mathcal{I},a}(q; \ell))_{a \in A}$$

with

$$c_{\mathcal{I},a}(q; \ell) = (q_a - q_a^-, q_a^+ - q_a)$$

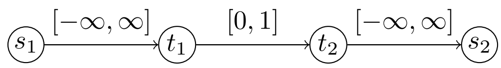

FIGURE 1. The graph G of Example 3.1

and $c_{\mathcal{E}}$ stays the same as in Section 2, i.e.,

$$c_{\mathcal{E}}(x, s; \ell) = c_{\mathcal{E}}(x; \ell) = (c_{\mathcal{E},u}(q; \ell))_{u \in V}$$

with

$$c_{\mathcal{E},u}(q; \ell) = \sum_{a \in \delta^{\text{out}}(u)} q_a - \sum_{a \in \delta^{\text{in}}(u)} q_a - \sigma_u \ell_u.$$

Note that checking the feasibility of a nomination $\ell \in N$ w.r.t. Conditions (1) of this section is a standard ℓ-transshipment problem; see Chapter 11 of the book [51].

In contrast to Section 2, we will see at the end of this section that a nomination may be infeasible w.r.t. given flow bounds. Hence, infeasible bookings may also exist. Additionally, for a feasible nomination there may exist a component-wise smaller nomination which is infeasible. To make this more concrete, we consider the following example.

Example 3.1. Let $G = (V, A)$ be a directed graph with nodes $V = \{s_1, s_2, t_1, t_2\}$ and arcs $A = \{(s_1, t_1), (t_1, t_2), (t_2, s_2)\}$. The nodes s_1, s_2 are entry nodes and t_1, t_2 are exit nodes. Furthermore, we set the flow bounds of the arcs (s_1, t_1) and (t_2, s_2) to $[-\infty, \infty]$ and for the remaining arc (t_1, t_2) to $[0, 1]$.

Then, one can show that the nomination

$$\ell_1 := (s_1, t_1, t_2, s_2)^\top = (5, 5, 5, 5)^\top$$

is feasible, i.e., $\ell \in F_N$. But the component-wise smaller nomination

$$\ell_2 := (s_1, t_1, t_2, s_2)^\top = (4, 0, 4, 0)^\top$$

is infeasible.

Thus, Example 3.1 leads to the following lemma.

Lemma 3.2. *The feasibility of a nomination $\ell \in F_N$ does not guarantee, in general, the feasibility of every component-wise smaller nomination $\tilde{\ell} \leq \ell$.*

Despite the previous result, the set of feasible nominations is still convex.

Lemma 3.3. *The set of feasible nominations F_N is convex.*

Proof. Let ℓ and $\tilde{\ell}$ be feasible nominations, i.e., $\ell, \tilde{\ell} \in F_N$ with corresponding flows q and $\tilde{q}$ that satisfy Conditions (3) and (4). Additionally, let λ be in $[0, 1]$. Then, $\lambda\ell + (1 - \lambda)\tilde{\ell} \in N$ is valid because $\lambda\ell, (1 - \lambda)\tilde{\ell} \in \mathbb{R}^{V_b}_{\geq 0}$ and

$$\sigma^\top(\lambda\ell + (1 - \lambda)\tilde{\ell}) = \lambda\sigma^\top\ell + (1 - \lambda)\sigma^\top\tilde{\ell} = \lambda 0 + (1 - \lambda)0 = 0$$

holds. Furthermore,

$$\begin{aligned}
&\lambda\sigma_u\ell_u + (1 - \lambda)\sigma_u\tilde{\ell}_u \\
&= \left(\sum_{a \in \delta^{\text{out}}(u)} \lambda q_a - \sum_{a \in \delta^{\text{in}}(u)} \lambda q_a \right) + \left(\sum_{a \in \delta^{\text{out}}(u)} (1 - \lambda)\tilde{q}_a - \sum_{a \in \delta^{\text{in}}(u)} (1 - \lambda)\tilde{q}_a \right) \\
&= \sum_{a \in \delta^{\text{out}}(u)} (\lambda q_a + (1 - \lambda)\tilde{q}_a) - \sum_{a \in \delta^{\text{in}}(u)} (\lambda q_a + (1 - \lambda)\tilde{q}_a)
\end{aligned}$$

holds for all $u \in V$ and thus $\lambda q + (1 - \lambda)\tilde{q}$ satisfies Constraint (3). Moreover, the relation $q_a^- \leq \lambda q + (1 - \lambda)\tilde{q} \leq q_a^+$ is valid because q and $\tilde{q}$ satisfy the flow bounds (4). Consequently, $\lambda\ell + (1 - \lambda)\tilde{\ell}$ is a feasible nomination. □

Lemma 3.3 implies the following corollary.

Corollary 3.4. The set of feasible nominations F_N is connected and star-shaped w.r.t. every point $x_0 \in F_N$.

Despite the set of feasible nominations is convex, connected, and star-shaped, it is in general not conic.

Lemma 3.5. *Let the flow bounds $q_a^- \leq q_a^+, a \in A$, be finite and assume that a feasible nonzero nomination $\ell \neq 0 \in F_N$ exists. Then, the set of feasible nominations F_N is not conic.*

Proof. Let $\ell \in F_N$ be a feasible nonzero nomination. Then, the corresponding flows satisfying Constraints (3) and (4) contain at least one nonzero arc flow. We can assume w.l.o.g. that the considered flows are nonnegative. Thus, scaling the nonzero nomination ℓ by a parameter $\lambda > 1$, increases at least one arc flow. Due to this and the finite flow bounds, we can scale ℓ by $\tilde{\lambda} \in \mathbb{R}_{>0}$ such that $\tilde{\lambda}\ell$ is feasible and for each $\varepsilon > 0$, the nomination $(\tilde{\lambda} + \varepsilon)\ell$ is infeasible. Hence, the set F_N of feasible nominations is not conic. □

Moreover, the set of feasible nominations is bounded if we consider finite flow bounds.

Lemma 3.6. *If the flow bounds $q_a^- \leq q_a^+$ are finite for all $a \in A$, then the set of feasible nominations F_N is bounded.*

Proof. We assume that the set of feasible nominations is unbounded and consequently, a feasible nomination $\ell \in F_N$ with $\sum_{u \in V_+} \ell_u > \sum_{a \in A} q_a^+$ exists. We assume w.l.o.g. that the corresponding arc flows are nonnegative. Hence, from Constraint (3) it follows that at least one arc flow violates its upper flow bound because in the considered nomination the injected flow is larger than the aggregated upper arc flow bounds. This is a contradiction to the feasibility of ℓ. □

After analyzing the feasibility of nominations, we now turn to the feasibility of bookings. In contrast to nominations, a feasible booking implies the feasibility of each component-wise smaller booking.

Lemma 3.7. *Let $b \in F_B$ be a feasible booking. Then, each booking $\tilde{b} \leq b$ is feasible. Furthermore, the set of feasible bookings F_B is star-shaped w.r.t. the zero booking.*

Proof. Let b be a feasible booking and $\tilde{b} \in B$ a booking with $\tilde{b} \leq b$. Consequently, $N(\tilde{b}) = \{\ell \in N : \ell \leq \tilde{b}\} \subseteq N(b)$ holds. Thus, the feasibility of the booking b implies the feasibility of $\tilde{b}$. From this it follows that the set F_B of feasible bookings is star-shaped w.r.t. the zero booking. □

Furthermore, we know that the set of feasible bookings is connected due to Lemma 3.7.

Corollary 3.8. The set of feasible bookings F_B is connected.

In analogy to the case of nominations, we can show that the set of feasible bookings is in general not conic.

Corollary 3.9. Let the flow bounds $q_a^- \leq q_a^+$, $a \in A$, be finite. Assume further that a feasible booking b with a b-compliant nonzero nomination $\ell \in F_N$ exists. Then, the set of feasible booking F_B is not conic.

Proof. From the proof of Lemma 3.5 it follows that $\lambda > 0$ exists so that $\lambda\ell$ is infeasible. Consequently, the set of bookings B is not conic. □

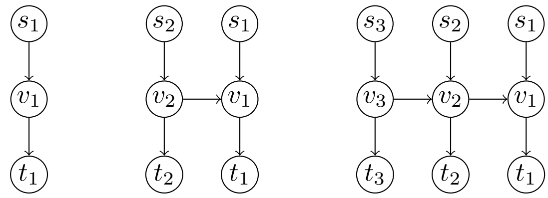

FIGURE 2. The H-networks H_1, H_2, H_3

With the help of an example, we now show that the set of all feasible bookings F_B is nonconvex in contrast to the set of feasible nominations F_N; see Lemma 3.3.

Definition 3.10 (H-networks)**.** The family of H-networks $H_n = (V_n, A_n)$ is defined by

$$H_1 := (V_1, A_1), \quad V_1 = \{s_1, v_1, t_1\}, \quad A_1 = \{(s_1, v_1), (v_1, t_1)\}$$

and $H_n := (V_n, A_n)$, $n \geq 2$, with

$$V_n = V_{n-1} \cup \{s_n, v_n, t_n\}, \quad A_n = A_{n-1} \cup \{(s_n, v_n), (v_n, t_n), (v_n, v_{n-1})\}.$$

See Figure 2 for the networks H_1, H_2, H_3. The nodes s_i are entry nodes, t_i are exit nodes, and v_i are inner nodes. The family of H-networks is also considered in [20] and in the chapter [25] of the book [35].

Example 3.11. We now consider the network H_2 and only impose a lower flow bound of zero of arc (v_2, v_1). All other flow bounds are formally set to $[-\infty, +\infty]$. One can show that

$$b_1 := (b_{s_2}, b_{s_1}, b_{t_2}, b_{t_1})^\top = (2, 2, 0, 2)^\top$$

and

$$b_2 := (b_{s_2}, b_{s_1}, b_{t_2}, b_{t_1})^\top = (2, 0, 2, 0)^\top$$

are feasible bookings, i.e., $b_1, b_2 \in F_B$. Consider now the convex combination b_3 with convex coefficient $\lambda = 1/2$, i.e.,

$$b_3 := (b_{s_2}, b_{s_1}, b_{t_2}, b_{t_1})^\top = (2, 1, 1, 1)^\top.$$

Obviously, the nomination

$$(b_{s_2}, b_{s_1}, b_{t_2}, b_{t_1})^\top = (0, 1, 1, 0)^\top$$

is b_3-compliant but *not* feasible.

Let us note at this point that a feasible booking, in contrast to a feasible nomination, does not need to be balanced.

Example 3.11 leads to the following theorem.

Theorem 3.12. *The feasible set of bookings F_B is, in general, nonconvex.*

Note this means that even a linear gas physics or engineering model may lead to a nonconvex set of feasible bookings.

Remark 3.13. For arbitrary $H_n = (V_n, A_n), n \geq 2$, we see that the following holds: If $b \in F_B$ is a feasible booking with $b_{t_k} > 0$ it follows $b_{s_j} = 0$ for all $j < k$. Thus, an exit node t_k, $k \geq 2$, can exclude every entry node s_j, $j < k$, from the market. Consider now for a moment the multicriteria optimization problem for which the feasible region is given by B. Moreover, the $|V_n|$ objective functions f_u, $u \in V_n$, are given by e_u, $u \in V_n$, with e_u being the uth unit vector; see, e.g., [16] for general multicriteria optimization. Then, from the above discussion and Example 3.11 it follows that the ideal point (in the sense of multicriteria optimization) is not bookable.

TABLE 2. Summary about properties of F_N and F_B w.r.t. gas transport model (3)–(4)

Properties	Gas transport constraints (3)–(4)
Bounded F_N	✓, see Lemma 3.6
Bounded F_B	×, see Lemma 3.14
Convex F_N	✓, see Lemma 3.3
Convex F_B	×, see Example 3.11
Connected F_N	✓, see Corollary 3.4
Connected F_B	✓, see Corollary 3.8
Star-shaped F_N	✓, see Corollary 3.4
Star-shaped F_B	✓, see Lemma 3.7
Conic F_N	×, see Lemma 3.5
Conic F_B	×, see Corollary 3.9

Furthermore, the set of feasible bookings is unbounded.

Lemma 3.14. *If the set of feasible bookings F_B is nonempty, then it is unbounded.*

Proof. The zero nomination is booking-compliant for every booking. Due to $F_B \neq \emptyset$, the zero nomination is feasible. Consequently, for each node $u \in V$ and nonnegative value M the booking b with $b_u = M$ and $b_v = 0, v \in V, v \neq u$, is feasible because the zero nomination is the only booking-compliant nomination for b. □

We note that for gas transport with flow bounds, the set of feasible bookings is unbounded in contrast to the set of feasible nominations; see Lemma 3.6 and 3.14. This is due to the definition of a feasible booking that only requires the feasibility of every balanced and component-wise smaller nomination. Consequently, bookings exist that only contain a single feasible booking-compliant nomination and scaling this booking does not change the set of balanced and booking-compliant nominations.

With the help of the following example, we show that even in the case of linear constraints of gas transport like (3) and (4) the set of feasible nominations and bookings can be empty. We consider the graph H_1. Additionally, we set the lower and upper flow bounds of arc (s_1, v_1) to 1 and of arc (v_1, t_1) to 2. For a given nomination $\ell \in N$ the flows q satisfying Conditions (3) are unique because G is a tree. Furthermore, the flow q_a on each arc $a \in A$ equals ℓ_{t_1}. Thus, no feasible nomination for G exists due to the chosen lower and upper arc flow bounds. Especially, the zero nomination, which is always b-compliant, is infeasible. Consequently, the set of feasible bookings is empty.

Finally, we summarize the results for a gas transport model using capacitated linear flows in Table 2.

4. A Nonlinear Flow Model for Passive Networks

We now extend the model of the last section to a more realistic model of gas physics by introducing a bounded pressure variable p_u for every node $u \in V$. Additionally, the pressure levels are coupled to arc flows. Hence, for a nomination $\ell \in N$ the Constraints (1) are given by (3), (4), and the classical Weymouth pressure drop conditions

$$p_v^2 = p_u^2 - \Lambda_a \, |q_a| \, q_a \quad \text{for all } a = (u, v) \in A, \tag{5}$$

where $\Lambda_a > 0$ is a constant for every arc $a \in A$. Furthermore, the pressures are bounded, i.e.,

$$0 < p_u^- \leq p_u \leq p_u^+ \quad \text{for all } u \in V. \tag{6}$$

Consequently, the Constraints (1) are represented by

$$c_{\mathcal{I}}(x,s;\ell) = c_{\mathcal{I}}(x;\ell) = \begin{pmatrix} (c_{\mathcal{I},u}(q;\ell))_{u\in V} \\ (c_{\mathcal{I},a}(q;\ell))_{a\in A} \end{pmatrix}$$

with

$$c_{\mathcal{I},u}(q;\ell) = (p_u - p_u^-, p_u^+ - p_u)$$

and the arc flow bounds

$$c_{\mathcal{I},a}(q;\ell) = (q_a - q_a^-, q_a^+ - q_a)$$

as well as

$$c_{\mathcal{E}}(x,s;\ell) = c_{\mathcal{E}}(x;\ell) = \begin{pmatrix} (c_{\mathcal{E},u}(q;\ell))_{u\in V} \\ (c_{\mathcal{E},a}(q;\ell))_{a\in A} \end{pmatrix}$$

with the flow conservation

$$c_{\mathcal{E},u}(q;\ell) = \sum_{a\in\delta^{\text{out}}(u)} q_a - \sum_{a\in\delta^{\text{in}}(u)} q_a - \sigma_u \ell_u$$

and

$$c_{\mathcal{E},a}(q;\ell) = p_u^2 - p_v^2 - \Lambda_a |q_a| q_a.$$

We now analyze the feasibility of nominations and bookings in this extended setting. In contrast to Sections 2 and 3, the set of feasible nominations F_N is now, in general, nonconvex. This follows from a small counterexample in Section 5.1 of [24].

Lemma 4.1. *The set of feasible nominations F_N is, in general, nonconvex.*

Despite the nonconvexity of the set of feasible nominations, we can guarantee that the set of feasible nominations is star-shaped w.r.t. the zero nomination under certain pressure and flow bound requirements. The main idea behind the proof is the following observation: When we fix the pressure at one node, then decreasing the flow to another node will also decrease the pressure drops along this path.

Lemma 4.2. *Suppose that $q_a^- \leq 0 \leq q_a^+$, $a \in A$, and $\bigcap_{u\in V}[p_u^-, p_u^+] \neq \emptyset$ holds. Then, the set of feasible nominations F_N is star-shaped w.r.t. the zero nomination.*

Proof. Let $\ell \in F_N$ be a feasible nomination with corresponding flow q satisfying Conditions (3) and (4). Additionally, let $p_u \in [p_u^-, p_u^+]$, $u \in V$, be the corresponding pressure levels satisfying Condition (5) and let $\lambda \in [0,1]$. We now show that F_N is star-shaped w.r.t. the zero nomination by proving that $\lambda\ell$ is a feasible nomination for any $\lambda \in [0,1]$. To this end, we consider the nomination $\lambda\ell$ with corresponding flows λq. The latter satisfies $q_a^- \leq \lambda q_a \leq q_a^+$ for every arc $a \in A$, because q satisfies the flow bounds, the requirement $q_a^- \leq 0 \leq q_a^+$ for all $a \in A$ holds, and $\lambda \in [0,1]$. We now have to find feasible pressure levels for the nomination $\lambda\ell$. From Theorem 7.1 in [34] it follows that we can compute an assignment $\tilde{p}$ of the pressure variables that satisfies Condition (5) with $\tilde{p}_u \leq p_u^+$ for all $u \in V$ and such that at least one node $u \in V$ satisfies $\tilde{p}_u = p_u^+$. We assume w.l.o.g. that the pressure level of the arbitrary node w is at its upper bound, i.e., $\tilde{p}_w = p_w^+$ holds.

We now contrarily assume that pressure levels $\tilde{p}$ do not satisfy the pressure bounds at each node. Due to the construction of $\tilde{p}$, the pressure level at every node satisfies its upper pressure bound. Due to this and the infeasibility of $\tilde{p}$, a node $v \in V$ with $\tilde{p}_v < p_v^-$ exists. We can further assume that $\lambda \in (0,1]$ holds, because for $\lambda = 0$ we obtain the zero nomination, which is feasible with zero arc flows and a constant pressure level $p_v = p \in \bigcap_{u\in V}[p_u^-, p_u^+] \neq \emptyset$ for every node $v \in V$. The existence of p is guaranteed by the requirements.

Case 1: The relation $\tilde{p}_v > \tilde{p}_w$ holds. This together with $\bigcap_{u \in V}[p_u^-, p_u^+] \neq \emptyset$, the assumption w.r.t. $\tilde{p}$, and $\tilde{p}_w = p_w^+$ leads to the following relations

$$p_v^+ \geq p_v^- > \tilde{p}_v > \tilde{p}_w = p_w^+ \geq p_w^-.$$

From the latter relations follows that $[p_v^-, p_v^+] \cap [p_w^-, p_w^+] = \emptyset$, which is a contradiction to $\bigcap_{u \in V}[p_u^-, p_u^+] \neq \emptyset$.

Case 2: The relation $\tilde{p}_v \leq \tilde{p}_w$ holds. We assume w.l.o.g. that $\tilde{p}_v$ is nonnegative (otherwise we would consider $|\tilde{p}_v|$), which again satisfies Condition (5), and thus, we are either in Case 1 or again in Case 2. Additionally, we assume w.l.o.g. that $P(w, v)$ is a directed path from w to v. Furthermore, $\tilde{p}$ satisfies Condition (5) and, thus,

$$\tilde{p}_w^2 - \sum_{a \in P(w,v)} \Lambda_a \, |\lambda q_a| \, \lambda q_a = \tilde{p}_v^2 \tag{7}$$

holds. Due to the last equation, $\tilde{p}_w \geq \tilde{p}_v \geq 0$, and $\lambda \in (0, 1]$, the relation

$$0 \leq \sum_{a \in P(w,v)} \Lambda_a \, |\lambda q_a| \, \lambda q_a \leq \sum_{a \in P(w,v)} \Lambda_a \, |q_a| \, q_a$$

is valid. This relation together with Equation (7), $\lambda \in (0, 1]$, $\tilde{p}_v \geq 0$, Condition (5), $(p_w^+)^2 = (\tilde{p}_w)^2 \geq p_w^2$, and the assumption leads to

$$\begin{aligned}
(p_v^-)^2 > \tilde{p}_v^2 &= \tilde{p}_w^2 - \sum_{a \in P(w,v)} \Lambda_a \, |\lambda q_a| \, \lambda q_a \\
&\geq p_w^2 - \sum_{a \in P(w,v)} \Lambda_a \, |\lambda q_a| \, \lambda q_a \geq p_w^2 - \sum_{a \in P(w,v)} \Lambda_a \, |q_a| \, q_a \\
&= p_v^2,
\end{aligned}$$

This is a contradiction to the feasibility of ℓ with corresponding feasible pressure levels $p_u, u \in V$. □

Note that a related result is given in Theorem 3.7 of [28]. Lemma 4.2 directly implies that the set of feasible nominations F_N is connected.

Corollary 4.3. The set of feasible nominations F_N is connected.

If the pressure requirement $\bigcap_{u \in V}[p_u^-, p_u^+] \neq \emptyset$ is not valid, then the set of feasible bookings is empty.

Lemma 4.4. *If $\bigcap_{u \in V}[p_u^-, p_u^+] = \emptyset$ is satisfied, then $F_B = \emptyset$ holds.*

Proof. Due to the requirement $\bigcap_{u \in V}[p_u^-, p_u^+] = \emptyset$, the zero nomination is not feasible, which directly shows the claim. □

The model of gas transport of this section is more restrictive than the model of Section 2. Thus, we can transfer Lemmas 3.5 and 3.6 to the nonlinear flow model on passive networks. Consequently, we know that the set of feasible nominations is not conic and that it is bounded. We now turn to the analysis of the bookings.

From Lemma 3.12, it follows that the set of feasible bookings is, in general, nonconvex. Furthermore, the statements in 3.7–3.9 and 3.14 are valid for the nonlinear flow model on passive networks and can be shown in analogy to Section 3. Consequently, the set of feasible bookings is connected and star-shaped w.r.t. the zero booking. Furthermore, the set of feasible bookings is unbounded if it is nonempty and examples with an empty set of feasible bookings exist; see Lemma 4.4.

We summarize the results for gas transport w.r.t. the nonlinear flow model on passive networks in Table 3. The main difference about the structural properties of nominations and bookings between the linear flow model of Sections 2 and 3 and the

TABLE 3. Summary about properties of F_N and F_B w.r.t. gas transport model (3)–(6)

Properties	Gas transport constraints (3)–(6)
Bounded F_N	✓, see Lemma 3.6
Bounded F_B	×, see Lemma 3.14
Convex F_N	×, see Lemma 4.1
Convex F_B	×, see Example 3.11
Connected F_N	✓, see Corollary 4.3
Connected F_B	✓, see Corollary 3.8
Star-shaped F_N	✓, see Lemma 4.2
Star-shaped F_B	✓, see Lemma 3.7
Conic F_N	×, see Lemma 3.5
Conic F_B	×, see Corollary 3.9

nonlinear flow model on passive networks is that the set of feasible nominations is convex in case of the linear flow model, which is not valid anymore in the nonlinear flow model.

5. A Mixed-Integer Nonlinear Flow Model for Active Networks

Besides nonlinear models of gas flow in pipes, real-world gas transport networks also comprise so-called active elements that can be controlled by the dispatcher. Examples for such devices are valves or compressors. Detailed descriptions of these active elements are, e.g., given in the chapters [19, 46] of the book [35]. For our nonlinear gas transport model, we focus on compressors as an example for active elements.

A compressor is represented by an arc $a = (u, v) \in A_{\mathrm{cs}} \subseteq A$ and we use the following simplified model (for more complicated models see, e.g., [48–50]). A compressor can be in bypass mode or active. In bypass mode, the in- and outflow pressures of the compressor are the same ($p_v = p_u$) and the flow through the compressor is arbitrary (within certain arc-specific bounds). If the compressor is active, it can compress the gas, i.e., the compressor increases the pressure. This capability is limited by lower and upper bounds on the obtained compression ratio, i.e.,

$$\frac{p_v}{p_u} \in [\varepsilon_a^-, \varepsilon_a^+] \quad \text{for all } a = (u, v) \in A_{\mathrm{cs}}$$

with $1 \leq \varepsilon_a^- \leq \varepsilon_a^+$. Both states of a compressor can be modeled by the constraints

$$\frac{p_v}{p_u} s_a \geq \varepsilon_a^- s_a + (1 - s_a)(p_u - p_v) \quad \text{for all } a = (u, v) \in A_{\mathrm{cs}}, \tag{8}$$

$$\frac{p_v}{p_u} s_a \leq \varepsilon_a^+ s_a + (1 - s_a)(p_u - p_v) \quad \text{for all } a = (u, v) \in A_{\mathrm{cs}}, \tag{9}$$

where the binary variable $s_a \in \{0, 1\}$, $a \in A_{\mathrm{cs}}$, equals 1 if only if the compressor is active. Otherwise the compressor is in bypass mode. In addition, the compressor has a nonnegative lower arc flow bound $\hat{q}^-$ in the active state for which we assume that $\hat{q}_a^- > q_a^-$ holds. (Otherwise we can neglect this lower arc flow bound of the compressor because of its standard arc flow bound.) We model this tightened lower flow bound of the compressor by modifying the lower arc flow bound constraint in (4) as follows:

$$q_a \geq (1 - s_a) q_a^- + s_a \hat{q}_a^-. \tag{10}$$

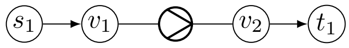

FIGURE 3. The graph of Example 5.1

Consequently, the Constraints (1) are given by

$$c_{\mathcal{I}}(x, s; \ell) = \begin{pmatrix} (c_{\mathcal{I},u}(q; \ell))_{u \in V} \\ (c_{\mathcal{I},a}(q; \ell))_{a \in A} \end{pmatrix}$$

with

$$c_{\mathcal{I},u}(q; \ell) = (p_u - p_u^-, p_u^+ - p_u)$$

and

$$c_{\mathcal{I},a}(s; q; \ell) = \begin{pmatrix} (s_a(p_v/p_u - \varepsilon_a^-) - (1 - s_a)(p_u - p_v))_{a=(u,v) \in A_{\text{cs}}} \\ (s_a(\varepsilon_a^+ - p_v/p_u) + (1 - s_a)(p_u - p_v))_{a=(u,v) \in A_{\text{cs}}} \\ (q_a - (1 - s_a)q_a^- - s_a \hat{q}^-)_{a \in A_{\text{cs}}} \\ (q_a - q_a^-)_{a \in A \setminus A_{\text{cs}}} \\ (q_a^+ - q_a)_{a \in A \setminus A_{\text{cs}}} \end{pmatrix}.$$

Additionally, we have the constraints

$$c_{\mathcal{E}}(x, s; \ell) = c_{\mathcal{E}}(x; \ell) = \begin{pmatrix} (c_{\mathcal{E},u}(q; \ell))_{u \in V} \\ (c_{\mathcal{E},a}(q; \ell))_{a \in A \setminus A_{\text{cs}}} \end{pmatrix}$$

with the flow conservation equations

$$c_{\mathcal{E},u}(q; \ell) = \sum_{a \in \delta^{\text{out}}(u)} q_a - \sum_{a \in \delta^{\text{in}}(u)} q_a - \sigma_u \ell_u$$

and the pressure drop conditions

$$c_{\mathcal{E},a}(q; \ell) = p_u^2 - p_v^2 - \Lambda_a \, |q_a| \, q_a.$$

We again analyze the set of feasible nominations and bookings in this extended setting. In contrast to Sections 2–4, the set of feasible nominations F_N is, in general, not connected anymore, which we will show by the following example.

Example 5.1. We consider the graph $G = (V, A)$ with nodes $V = \{s_1, v_1, v_2, t_1\}$, where s_1 is an entry, v_1, v_2 are inner nodes, and t_1 is an exit. Additionally, the graph contains three arcs (s_1, v_1), (v_1, v_2), and (v_2, t_1), where the arc (v_1, v_2) represents a compressor. A graphical representation is given in Figure 3. We set the pressure bounds to $[2, 2]$ for node s_1 and to $[1, 2]$ for the remaining nodes. Furthermore, the lower and upper bounds for the compression ratio are given by $[\varepsilon^-, \varepsilon^+] = [2, 3]$ and the pressure drop coefficient Λ_a equals 0.5 for every arc $a \in A \setminus A_{\text{cs}}$. We neglect flow bounds in this example. The graph G is a tree with one entry and one exit. Due to this and Definition 2.2, a nomination in G equals $(\ell, \ell), \ell \in \mathbb{R}_{\geq 0}$, with the arc flows $q_a = \ell$, $a \in A$, where ℓ is the amount of gas which is injected at the entry and withdrawn at the exit of the network. If the compressor is in bypass mode, then each feasible nomination has to satisfy the pressure Constraints (5) and (6), i.e.,

$$p_{s_1} = 2, \quad p_{v_1} = 2 - 0.5\ell^2 = p_{v_2} \geq 1, \quad p_{t_1} = p_{v_2} - 0.5\ell^2 = 2 - \ell^2 \geq 1.$$

Thus, the set of feasible nominations is $\{(\ell, \ell) : \ell \in [0, 1]\}$ in this case. If the compressor is active, then each feasible nomination $(\ell, \ell), \ell \in \mathbb{R}_{\geq 0}$, has to satisfy

$$p_{s_1} = 2, \; p_{v_1} = 2 - 0.5\ell^2 \geq 1, \; 2 \leq \frac{p_{v_2}}{p_{v_1}} \leq 3, 1 \leq p_{v_2} \leq 2, \; p_{t_1} = p_{v_2} - 0.5\ell^2 \geq 1.$$

and consequently, only the nomination $(\sqrt{2}, \sqrt{2})$ is feasible. Hence, the set of feasible nominations is $F_N = \{(\ell, \ell) : \ell \in [0, 1]\} \cup \{(\sqrt{2}, \sqrt{2})\}$, which is not connected.

Example 5.1 leads to the following lemma.

Lemma 5.2. *The set of feasible nominations F_N is, in general, not connected—even if no arc flow bounds are considered.*

We now present another example, which also proves Lemma 5.2. While in Example 5.1 the set of feasible nominations is not connected due to bounds on the compression ratio, in the next example the feasible set of nominations is disconnected due to the presence of a lower arc flow bound of the compressor.

Example 5.3. We again consider the network $G = (V, A)$ of the last example. We modify the lower and upper pressure bounds to $[0.875, 2]$ for v_1 and to $[1, 3]$ for v_2 and t_1. Furthermore, the lower and upper bounds for the compression ratio are set to $[1, 3]$. The set of feasible nominations is $F_N = \{(\ell, \ell) : \ell \in [0, 1.5]\}$ because each feasible nomination $(\ell, \ell), \ell \in \mathbb{R}_{\geq 0}$, has to satisfy the following pressure constraints

$$p_{s_1} = 2, \quad p_{v_1} = 2 - 0.5\ell^2 \geq 0.875,$$
$$1 \leq \frac{p_{v_2}}{p_{v_1}} \leq 3, \quad 1 \leq p_{v_2} \leq 3, \quad p_{t_1} = p_{v_2} - 0.5\ell^2 \geq 1.$$

We note that the set of feasible nominations is connected and that $p_{v_2}/p_{v_1} = 1$ corresponds to the bypass mode. If the compressor is inactive, the nominations $\{(\ell, \ell) : \ell \in [0, 1]\}$ are feasible and with the help of the compressor the remaining nominations of F_N are feasible. We now add the lower flow bound $\hat{q}^- = 1.25$ for the compressor, which comes into play if the compressor is active. Consequently, the set of feasible nominations is $F_N = \{(\ell, \ell) : \ell \in [0, 1] \cup [1.25, 1.5]\}$, which is not connected. Hence, we see that the lower flow bound of the compressor may also lead to a disconnected set of feasible nominations.

From Lemma 5.2 it follows that the set of feasible nominations is, in general, neither conic, star-shaped, nor convex.

Corollary 5.4. The set of feasible nominations F_N is, in general, neither conic, star-shaped, nor convex.

Furthermore, from Lemma 3.6 it follows that the set F_N of feasible nominations is bounded.

We now turn to the analysis of the bookings. The nonlinear flow model on passive networks is a special case of the considered nonlinear flow model on active networks. Hence, we can conclude from Section 4 that the set of feasible bookings is, in general, nonconvex and that examples with an empty set of feasible bookings exist. Additionally, we can prove in analogy to Section 4 that the set of feasible bookings is, in general, connected and star-shaped w.r.t. the zero booking. Moreover, the set of feasible bookings is unbounded if it is nonempty.

We summarize the results for gas transport w.r.t. the nonlinear flow model on active networks in Table 4. The main difference about the structural properties of nominations and bookings between the nonlinear flow model on passive and on active networks is that the set of feasible nominations is connected and star-shaped on passive networks, which is not the case anymore on active networks.

6. Conclusion

In this work, we analyzed the structural properties of the set of feasible nominations and feasible bookings in the European entry-exit gas market system. We presented a formal definition of (feasible) bookings and then studied whether this set is bounded, convex, connected, conic, and star-shaped—which are all important properties if one wants to optimize over this set. We carried out the analysis for different gas flow models on a network, ranging from a simple capacitated linear flow model to a mixed-integer nonlinear model of an active network. The results

TABLE 4. Summary about properties of F_N and F_B w.r.t. gas transport model (3)–(6), (8)– (10)

Properties	Gas transport constraints (3)–(6), (8)–(10)
Bounded F_N	✓, see Lemma 3.6
Bounded F_B	×, see Lemma 3.14
Convex F_N	×, see Corollary 5.4
Convex F_B	×, see Example 3.11
Connected F_N	×, see Example 5.1
Connected F_B	✓, see Corollary 3.8
Star-shaped F_N	×, see Corollary 5.4
Star-shaped F_B	✓, see Lemma 3.7
Conic F_N	×, see Corollary 5.4
Conic F_B	×, see Corollary 3.9

TABLE 5. Summary about properties of F_N and F_B w.r.t. different gas transport models

	Gas transport constraints			
Properties	(3)	(3), (4)	(3)–(6)	(3)–(6), (8)–(10)
Bounded F_N	×	✓	✓	✓
Bounded F_B	×	×	×	×
Convex F_N	✓	✓	×	×
Convex F_B	✓	×	×	×
Connected F_N	✓	✓	✓	×
Connected F_B	✓	✓	✓	✓
Star-shaped F_N	✓	✓	✓	×
Star-shaped F_B	✓	✓	✓	✓
Conic F_N	✓	×	×	×
Conic F_B	✓	×	×	×

are summarized in Table 5. It turns out that some of the results on the feasible set of bookings are rather counter-intuitive. For instance, one can see that all models (except for the very simplified linear one without arc capacities) lead to nonconvex sets of feasible bookings. This is remarkable because this already happens for the model that only uses a very simple linear flow model with arc capacities. It also indicates that it can be expected that optimizing over these sets is hard. This is in line with results from the literature like in [32], where it is shown that checking the feasibility of a booking is a coNP-hard problem on general graphs—even for linear flow models. However, the results in [45] imply that the same problem is easy for nonlinear flow models on trees. One interesting question for future research thus is to exactly draw the line between the easy and the hard cases. The analysis of feasible bookings in the context of instationary gas flow models is also part of our future work. However, with respect to stationary models, it can be seen in Table 5 that the only desirable properties of bookings that still hold in the nonlinear flow model with active elements are purely based on the nature of feasible bookings and thus do not depend on the chosen physical and technical models of gas transport.

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Compliance with Ethical Standards

The authors declare that they have no conflict of interest.

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Article 3

Deciding feasibility of a booking in the European gas market on a cycle is in P for the case of passive networks

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RESEARCH ARTICLE

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Deciding feasibility of a booking in the European gas market on a cycle is in P for the case of passive networks

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Abstract

We show that the feasibility of a booking in the European entry-exit gas market can be decided in polynomial time on single-cycle networks that are passive, i.e., do not contain controllable elements. The feasibility of a booking can be characterized by solving polynomially many nonlinear potential-based flow models for computing so-called potential-difference maximizing load flow scenarios. We thus analyze the structure of these models and exploit both the cyclic graph structure as well as specific properties of potential-based flows. This enables us to solve the decision variant of the nonlinear potential-difference maximization by reducing it to a system of polynomials of constant dimension that is independent of the cycle's size. This system of fixed dimension can be handled with tools from real algebraic geometry to derive a polynomial-time algorithm. The characterization in terms of potential-difference maximizing load flow scenarios then leads to a polynomial-time algorithm for deciding the feasibility of a booking. Our theoretical results extend the existing knowledge about the complexity of deciding the feasibility of bookings from trees to single-cycle networks.

KEYWORDS

bookings, computational complexity, cycle, European entry-exit market, gas networks, potential-based flows

1 | INTRODUCTION

During the last decades, the European gas market has undergone ongoing liberalization [10–12], resulting in the so-called entry-exit market system [22]. The main goal of this market re-organization is the decoupling of trading and actual gas transport. To achieve this goal within the European entry-exit market, gas traders interact with transport system operators (TSOs) via bookings and nominations. A booking is a capacity-right contract in which a trader reserves a maximum injection or withdrawal capacity at an entry or exit node of the TSO's network. On a day-ahead basis, these traders are then allowed to nominate an actual load flow up to the booked capacity. To this end, the traders specify the actual amount of gas to be injected to or withdrawn from the network such that the total injection and withdrawal quantities are balanced. On the other hand, the TSO is responsible for the transport of the nominated amounts of gas. By having signed the booking contract, the TSO guarantees that the nominated amounts can actually be transported through the network. More precisely, the TSO needs to be able to transport every set of nominations that complies with the signed booking contracts. Thus, an infinite number of possible nominations must be anticipated and checked for feasibility when the TSO accepts bookings. As a consequence, the entry-exit market decouples trading and transport. However, it also introduces many new challenges, e.g., the checking of feasibility of bookings or the computation of bookable capacities on the network [13, 26].

A large branch of research considers the feasibility of nominations, as well as the physics and the optimal control of gas networks w.r.t. single nominations. Early works such as [28] or [8] study the physical properties of pipe networks. In particular, it is shown that in connected pressure-based networks the flow corresponding to a given load scenario is unique (given that the pressure at an arbitrary node is fixed). This result holds more generally for a potential-based flow model; see, e.g., [31]. Such a potential-based flow model is also used in [19] as an abstract model that approximates, among others like water or lossless direct current (DC) power flow, the physics of stationary flows in gas networks. More generally, the study of gas transport and the feasibility of nominations has been researched from many different optimization perspectives. For instance, in [9] and [4], the authors study the cost-optimal transport of gas in the Belgian network before and after the market liberalization. An extension of the simplex algorithm is proposed to solve the problem for the case in which gas physics are approximated by piecewise-linear functions, enabling mixed-integer linear programming (MILP) techniques to be used. MILP approaches can also be found, e.g., in [16, 17, 27]. On the other hand, purely continuous and highly accurate nonlinear optimization (NLP) models are discussed, e.g., in [33]. The combination of both worlds leads to challenging mixed-integer nonlinear models that are tackled, e.g., in [15, 23]. For an in-depth overview of optimization problems in gas networks, we also refer to the recent survey [30] as well as the book [24] and the references therein.

In contrast to the very rich literature on nominations, there is much less literature on checking the feasibility of a booking. First mathematical analyses of bookings are presented in the PhD theses [21, 34]. Moreover, the early technical report [14] discusses the reservation-allocation problem, which is highly related to the feasibility of bookings in the European entry-exit gas market. Deciding the feasibility of a booking can also be seen as an adjustable robust feasibility problem [6], where the set of booking-compliant nominations is the uncertainty set. Exploiting this perspective, the authors of [3] propose set containment techniques to decide robust feasibility and infeasibility with an application to the Greek gas transport network. With an application to a tree-shaped hydrogen network, the problem of robust discrete arc sizing is discussed in [29]. In [2], the uncertainty of physical parameters is considered. On the other hand, structural properties of the sets of feasible nominations and bookings such as nonconvexity and star-shapedness are discussed in [32]. For networks consisting of pipes only, a characterization of feasible bookings is given in [25] by conditions on nominations with maximum potential difference in the network. Using a linear potential-based flow model, these nominations can be computed efficiently using linear programming. In the nonlinear case, the authors give a polynomial-time dynamic programming approach for deciding the feasibility of a booking, if the underlying network is a tree. For the general case, i.e., nonlinear potential-based physics and arbitrary network topologies, the complexity of deciding the feasibility of a booking is not yet clear and only exponential upper bounds are given in [21]. However, neither hardness results nor polynomial-time algorithms can be found in the literature for cases where the network is not a tree.

In the light of this literature, our contribution is as follows. We extend the knowledge on the hardness of the problem by showing that deciding the feasibility of a booking on single-cycle networks is in P. We analyze the structure of potential-difference maximizing nominations by exploiting the cyclic structure of the network as well as techniques specific to potential-based flow models. Interestingly, this allows us to reduce the task of checking the feasibility of a booking to checking the solvability of a system of polynomial equalities and inequalities in fixed dimension, where the latter does not depend on the size of the cycle. These systems of fixed dimension can then be tackled with tools from real algebraic geometry to derive a polynomial-time algorithm for deciding the feasibility of a booking.

The remainder of this article is structured as follows. In Section 2, the problem of checking the feasibility of a booking is formally defined. Section 3 collects notations and known results that are used in this work. In Section 4, we introduce a notion of so-called flow-meeting points in cycle networks and study properties of potential-difference maximizing nominations in Section 5. These results are then combined in Section 6 to derive a polynomial-time algorithm for deciding the feasibility of a booking on a cycle. Finally, we draw a conclusion and pose some open questions for future research in Section 7.

2 | PROBLEM DESCRIPTION

Before restricting ourselves to cycles, we first introduce the problem of verifying the feasibility of bookings for general networks. Thus, we model a gas network using a weakly connected directed graph $G = (V, A)$ with node set V and arc set A. The set of nodes is partitioned into the set V_+ of entry nodes, at which gas is supplied, the set V_- of exit nodes, where gas is withdrawn, and the set V_0 of the remaining inner nodes. The node types are encoded in a vector $\sigma = (\sigma_u)_{u \in V}$, given by

$$\sigma_u = \begin{cases} 1, & \text{if } u \in V_+, \\ -1, & \text{if } u \in V_-, \\ 0, & \text{if } u \in V_0. \end{cases}$$

In real-world gas networks, the arc set is typically partitioned into different types of arcs that correspond to different elements of the network, e.g., pipes, compressors, and control valves. However, we restrict our analysis to passive networks that consist of pipes only. We follow the notation and definitions of [32], which we briefly introduce in the following.

Definition. A *load* is a vector $\ell = (\ell_u)_{u \in V} \in \mathbb{R}^V_{\geq 0}$, with $\ell_u = 0$ for all $u \in V_0$. The set of load vectors is denoted by L.

A load vector thus corresponds to an actual situation at a single point in time by specifying the amount of gas ℓ_u that is supplied at $u \in V_+$ or withdrawn at $u \in V_-$. Since we only consider stationary flows, we need to impose that the supplied amount of gas equals the withdrawn amount, which leads to the definition of a nomination.

Definition. A *nomination* is a balanced load vector ℓ, i.e., $\sigma^\top \ell = 0$. The set of nominations is given by

$$N := \{\ell \in L : \sigma^\top \ell = 0\}.$$

A booking, on the other hand, is a load vector defining bounds on the admissible nomination values. More precisely, we have the following definition.

Definition. A *booking* is load vector $b \in L$. A nomination ℓ is called booking-compliant w.r.t. the booking b if $\ell \leq b$ holds, where "$\leq$" is meant componentwise throughout this article. The set of booking-compliant (or b-compliant) nominations is given by

$$N(b) := \{\ell \in N : \ell \leq b\}.$$

Next, we introduce the notion of feasibility for nominations and bookings. We model stationary gas flows using an abstract physics model based on the Weymouth pressure drop equation and potential flows; see, e.g., [19] or [25]. It consists of arc flow variables $q = (q_a)_{a \in A} \in \mathbb{R}^A$ and potentials on the nodes $\pi = (\pi_u)_{u \in V} \in \mathbb{R}^V_{\geq 0}$. We note that, in this context, potentials are linked to gas pressures at the nodes via $\pi_u = p_u^2$ for the case of horizontal pipes. An in-depth explanation for nonhorizontal pipes is given in [19].

Definition. A nomination $\ell \in N$ is *feasible* if a point (q, π) exists that satisfies

$$\sum_{a \in \delta^{\text{out}}(u)} q_a - \sum_{a \in \delta^{\text{in}}(u)} q_a = \sigma_u \ell_u, \qquad u \in V, \tag{1a}$$

$$\pi_u - \pi_v = \Lambda_a q_a |q_a|, \qquad a = (u, v) \in A, \tag{1b}$$

$$\pi_u \in [\pi_u^-, \pi_u^+], \qquad u \in V, \tag{1c}$$

where $\delta^{\text{out}}(u)$ and $\delta^{\text{in}}(u)$ denote the sets of arcs leaving and entering node $u \in V$, $\Lambda_a > 0$ is an arc-specific constant for any $a \in A$, and $0 < \pi_u^- \leq \pi_u^+$ are potential bounds for any $u \in V$.

Constraints (1a) ensure that flow is conserved at every node w.r.t. the nomination ℓ. For any $a = (u, v) \in A$, Constraint (1b) links the flow q_a to the difference $\pi_u - \pi_v$ of potentials at the endpoints of a. We note that flow can be negative, if it flows in the opposite direction of the orientation of the arc. Finally, due to technical restrictions of the network, the potentials need to satisfy bounds (1c). In a weakly connected network that only consists of pipes, the flow $q = q(\ell)$ corresponding to a given nomination $\ell \in N$ is unique since it is the optimal solution of a strictly convex minimization problem [28]. The potentials $\pi = \pi(\ell)$ are the corresponding dual variables and are unique as soon as a reference potential is fixed; see, e.g., [31]. The potentials are therefore unique up to shifts, which in particular implies that potential differences between nodes are unique for a given nomination ℓ. The feasibility of a given nomination can be checked using the approach described in [18]. In contrast, verifying the feasibility of a booking is less researched and much more difficult.

Definition. We say that a booking b is *feasible* if all booking-compliant nominations $\ell \in N(b)$ are feasible.

To assess the feasibility of a booking, by definition, a possibly infinite number of nominations need to be checked.

Remark. Deciding the feasibility of a booking can be seen as very special case of deciding the feasibility of an adjustable robust optimization problem with uncertainty set $N(b)$. Let us briefly highlight this relationship in this remark. In principle, for every booking-compliant nomination, we are allowed to adjust the corresponding flow and the corresponding potentials according to the feasibility system (1). However, the decision rule (in terms of adjustable robust optimization) is very special. Note again that, for a given nomination $\ell \in N(b)$, the resulting flow is uniquely determined and all potentials are uniquely determined if we fix a certain potential π_w at an arbitrarily chosen reference node w, e.g., if we set $\pi_w = \psi$ for a reference potential ψ. Thus, we face the adjustable robust problem in which the uncertainty set consists of all booking-compliant nominations and that can be formalized as

$$\forall \ell \in N(b) : \exists y^{\psi} \in Y : \pi_u^- \leq y_u^{\psi}(\ell) \leq \pi_u^+, \quad u \in V. \tag{2}$$

Here, Y corresponds to the ψ-parameterized set of decision rules, which map given nominations to node potentials, i.e., $y^{\psi} \in Y$ and $y^{\psi} : N(b) \to \mathbb{R}^V$. This, in particular, means that for a given nomination, the only choice is the reference pressure since all flows and potentials are uniquely determined afterward by (1).

Consequently, deciding the feasibility of a booking is equivalent to finding a specific decision rule in the ψ-parameterized family of functions Y. Note that the uncertainty is not given in a constraintwise way. Additionally, the decision rules must satisfy (1b), which has a nonlinear right-hand side that is nonsmooth in zero. Consequently, the decision rules are also nonlinear and nonsmooth in general. The related adjustable robust problem is thus a very special one that is, in general, not tractable in terms of adjustable robust optimization; see, e.g., [7] or the recent survey [35] as well as the references therein. One particular contribution of this article is that the problem-specific structure at hand is exploited so that the considered problem (which looks highly intractable at a first glance) can be solved efficiently. The further question on whether the developed techniques may be generalized to general adjustable robust flow problems is beyond the scope of this article.

In every network, the zero flow associated with the zero nomination is always feasible. It is achieved by having the same potential at every node. This, in particular, leads to the following assumption on the bounds of the potentials.

Assumption 1. *The potential bound intervals have a nonempty intersection, i.e.,*

$$\bigcap_{u \in V} [\pi_u^-, \pi_u^+] \neq \emptyset.$$

Since the zero nomination is always booking compliant, this assumption is required for having a feasible booking at all. Thus, the assumption is also required to allow for a reasonable study of deciding the feasibility of bookings.

It is shown in Theorem 10 of [25] that a feasible booking b can be characterized by constraints on the maximum potential differences between all pairs of nodes. Therefore, the authors introduce, for every fixed pair of nodes $(w_1, w_2) \in V^2$, the following problem

$$\varphi_{w_1 w_2}(b) := \max_{\ell, q, \pi} \quad \pi_{w_1} - \pi_{w_2} \tag{3a}$$

$$\text{s.t.} \quad \text{(1a), (1b)},$$

$$0 \leq \ell_u \leq b_u, \quad u \in V, \tag{3b}$$

where $\varphi_{w_1 w_2}$ is the corresponding optimal value function (depending on the booking b). Then, the booking b is feasible if and only if

$$\varphi_{w_1 w_2}(b) \leq \pi_{w_1}^+ - \pi_{w_2}^- \tag{4}$$

holds for every fixed pair of nodes $(w_1, w_2) \in V^2$. Hence, to verify the feasibility of a booking using this approach, it is necessary to solve the nonlinear and nonconvex global optimization problems (3). For tree-shaped networks, the authors give a polynomial-time dynamic programming algorithm for solving (3). As a consequence, verifying the feasibility of a booking on trees can be done in polynomial time, which can also be obtained by adapting the results of [32]. In this article, we show that (4) can still be decided in polynomial time on a single cycle.

3 | NOTATION AND BASIC OBSERVATIONS

Entry and exit nodes $v \in V_+ \cup V_-$ are called *active* if $\ell_v > 0$ holds. We denote by $V_+^> := \{v \in V_+ : \ell_v > 0\}$ and $V_-^> := \{v \in V_- : \ell_v > 0\}$ the set of active entries and exits, respectively.

Using directed graphs to represent gas networks is a modeling choice that allows us to interpret the direction of arc flows. However, the physical flow in a potential-based network is not influenced by the direction of the arcs. Thus, for $u, v \in V$, we introduce the so-called *flow-paths* $P := P(u, v) = (V(P(u, v)), A(P(u, v)))$ in which $V(P(u, v)) \subseteq V$ contains the nodes of the path from u to v in the undirected version of the graph G and $A(P(u, v)) \subseteq A$ contains the corresponding arcs of this path. Note that these flow-paths are not necessarily unique. For another pair of nodes $u', v' \in V$, we say that $P(u', v')$ is a *flow-subpath* of $P(u, v)$ if $P(u', v') \subseteq P(u, v)$, i.e., $V(P(u', v')) \subseteq V(P(u, v))$ and $A(P(u', v')) \subseteq A(P(u, v))$, and if $P(u', v')$ is itself a flow-path. In particular, this allows us to define an order on the nodes of a flow-path. For $P = P(u, v)$ and $u', v' \in P$, we define $u' \preccurlyeq_P v'$ if and only if a flow-subpath $P(u, u') \subseteq P(u, v')$.[1] If $u' \neq v'$ holds, we write $u' \prec_P v'$.

We now introduce the *characteristic function* of an arc $a = (u, v) \in A$. For any flow-path P, it is given by

$$\chi_a(P) := \begin{cases} 1, & \text{if } u \prec_P v, \\ -1, & \text{if } v \prec_P u, \\ 0, & \text{if } a \notin P. \end{cases}$$

Next, we adapt a classical result from linear flow models to construct a flow decomposition in a gas network.

Lemma 2. *Given $\ell \in N \setminus \{0\}$, let $\mathcal{P}_\ell := \{P(u, v) : u \in V_+^>, v \in V_-^>\}$ be the set of flow-paths in G with an active entry as start node and an active exit as end node. Then, a decomposition of the given flow $q = q(\ell)$ into path flows exists, such that*

$$q_a = \sum_{P \in \mathcal{P}_\ell} \chi_a(P)\, q(P), \quad a \in A, \tag{5}$$

where $q(P)$ is the nonnegative flow along the flow-path $P \in \mathcal{P}_\ell$.

Furthermore, we require that if $q_a > 0$ for $a \in A$ and $\chi_a(P) = -1$ for $P \in \mathcal{P}_\ell$, then $q(P) = 0$ holds. Similarly, if $q_a < 0$ for $a \in A$ and $\chi_a(P) = 1$ for $P \in \mathcal{P}_\ell$, then $q(P) = 0$ holds.

Proof. If $q_a < 0$ holds, then we replace arc $a = (u, v)$ by (v, u) and set $q_{(v,u)} = -q_{(u,v)}$. The resulting flow still corresponds to nomination ℓ. We now apply Theorem 3.5 of Chapter 3.5 of the book by Ahuja et al. [1]. Given Constraints (1b), the flow q cannot contain any cycle flows. As a consequence, we obtain a flow decomposition that satisfies all the properties. ∎

Observe that, by construction, the flow q and the path flows need to traverse arcs in the same direction. A direct consequence of the flow decomposition is that the nomination can be expressed as a function of the path flows.

Corollary 3. *For any $u \in V_+^>$, the condition*

$$\sum_{v \in V_-^>} q(P(u, v)) = \ell_u \tag{6}$$

and for any $v \in V_-^>$, the condition

$$\sum_{u \in V_+^>} q(P(u, v)) = \ell_v \tag{7}$$

is satisfied.

Next, we define the potential-difference function along a given flow-path.

Definition. Let $\ell \in N$ and a flow-path P be given. Then, the *potential-difference function* along P is given by

$$\Pi_P : \mathbb{R}^A \to \mathbb{R}, \quad \Pi_P(q) := \sum_{a \in P} \chi_a(P) \Lambda_a q_a |q_a|, \tag{8}$$

where $q = q(\ell)$.

As a consequence of Constraint (1b), for any node pair $u, v \in V$ and for any flow-path $P := P(u, v)$, the equation $\pi_u(\ell) - \pi_v(\ell) = \Pi_P(q(\ell))$ holds. We note that if the path P is directed from u to v, the potential-difference function simplifies to

$$\Pi_P(q) = \sum_{a \in P} \Lambda_a q_a |q_a|.$$

Since, we will mostly use directed paths in what follows, we state some properties that hold in this case.

Lemma 4. *For $u, v \in V$, let $P := P(u, v)$ be a directed path. Then, the following holds:*

(a) Π_P *is continuous.*

[1]For the ease of presentation, we also use the notation $u \in P = P(u, v)$ instead of $u \in V(P(u, v))$ or $a \in P$ instead of $a \in A(P(u, v))$, if it is clear from the context.

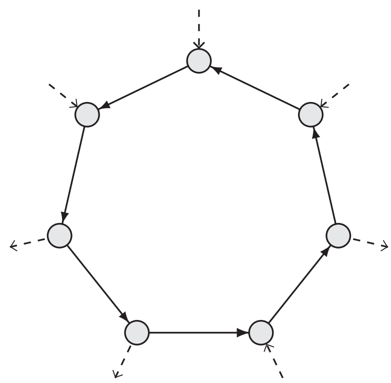

FIGURE 1 Example of a cyclic gas network. Dashed arcs to or from a node indicate entries or exits, respectively

(b) Π_P *is strictly increasing w.r.t. every component. That means, for q fixed except for one value* q_a, $a \in P$, Π_P *is increasing in* q_a.

(c) Π_P *is unbounded w.r.t. every component, i.e., for* $a \in P$,

$$\lim_{q_a \to -\infty} \Pi_P(q) = -\infty \quad \text{and} \quad \lim_{q_a \to \infty} \Pi_P(q) = \infty.$$

(d) Π_P *is additive w.r.t. the flow-path, i.e., for all* $v' \in P$,

$$\Pi_P = \Pi_{P(u,v')} + \Pi_{P(v',v)},$$

where $P = P(u, v') \cup P(v', v)$.

(e) $\Pi_P \geq 0$ *holds if and only if* $\pi_u \geq \pi_v$ *holds.*

4 | PROBLEM REDUCTION VIA FLOW-MEETING POINTS

In the remainder of this article, we restrict ourselves to a network that is a single cycle. A stylized example of a cyclic gas network is shown in Figure 1. A first observation is that in a potential-based flow model, there cannot be any cycling flow. Thus, flow in a cycle has to "meet" in at least one node. In this section, we show that the set of all feasible flows in Problem (3) can be restricted to flow along two different paths without changing direction along the way.

In a cycle, for every pair of nodes $u, v \in V$, exactly two flow-paths exist. We denote by $P^{\mathrm{l}}(u, v) = (V^{\mathrm{l}}(u, v), A^{\mathrm{l}}(u, v))$ the *left path* obtained when v is reached in counterclockwise direction from u. Similarly, $P^{\mathrm{r}}(u, v) = (V^{\mathrm{r}}(u, v), A^{\mathrm{r}}(u, v))$ is the *right path* obtained by using the clockwise direction. Moreover, $A = A^{\mathrm{l}}(u, v) \cup A^{\mathrm{r}}(u, v)$ holds. If it is clear from the context, we use previously introduced notations indexed by "l" (left) or "r" (right), when they have to be understood w.r.t. P^{l} or P^{r}.

It is not hard to observe that, given Constraints (1a) and (1b), the highest potential in G is attained at an entry node.

Lemma 5. *Let* $\ell \in N\backslash\{0\}$ *and* $o \in V_+$ *be an entry with highest potential. Then,* $\pi_o(\ell) \geq \pi_v(\ell)$ *holds for all* $v \in V$.

Given that no cycle flow is possible in a gas network, flow needs to change the direction along a single cycle. We now specify a node as flow-meeting point if arc flows from different directions "meet" at this node.

Definition. Let $\ell \in N\backslash\{0\}$ and $o \in V_+$ be an entry node with highest potential, i.e., $\pi_o(\ell) \geq \pi_v(\ell)$ for all $v \in V$. Then, $w \in V\backslash\{o\}$ is a flow-meeting point if there exist $u \in V^{\mathrm{l}}(o, w)$ adjacent to w that satisfies $\pi_u(\ell) > \pi_w(\ell)$ as well as $v \in V^{\mathrm{r}}(o, w)$ such that $\pi_v(\ell) > \pi_w(\ell)$ and $\pi_{v'}(\ell) = \pi_w(\ell)$ holds for all $v' \in V^{\mathrm{r}}(v, w)\backslash\{v\}$.

This definition is illustrated in Figure 2. Note that we choose the node $o \in V_+$ with highest potential to ensure that there is no flow through node o. If multiple entry nodes with highest potential exist, flow-meeting points are still well defined. In fact, as a direct consequence of Lemma 5, the definition of a flow-meeting point is independent of the choice of node o. By definition, the flow-meeting point w has nonzero flow entering on one arc and possibly zero flow on the other arc. Thus, w is necessarily an exit.

From Constraints (1a) and (1b), it directly follows that for every nonzero nomination at least one flow-meeting point exists. We note that there can be multiple flow-meeting points with different potentials. However, since every flow-meeting point is an exit, it is not hard to observe that the following result holds.

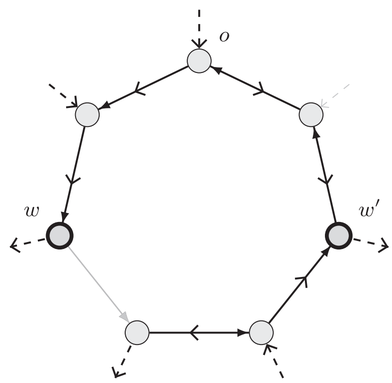

FIGURE 2 Flow directions and resulting flow-meeting points. Bold arcs indicate entry-exit activity and flow directions, whereas gray arcs indicate inactive nodes or zero arc-flow. In this example, exits w and w' are flow-meeting points

Lemma 6. *Let $\ell \in N\backslash\{0\}$ and w be a flow-meeting point with lowest potential. Then, $\pi_w(\ell) \leq \pi_v(\ell)$ holds for all $v \in V$.*

In the remainder of this section, we show that for fixed $(w_1, w_2) \in V^2$ there are optimal solutions of (3) with at most one flow-meeting point. More precisely, we prove that an optimal solution exists that has a special entry node $o \in V_+$, a special exit node $w \in V_-$, and has nonnegative flow from o to w.

Before we prove several auxiliary results, let us first make a notational comment. For $(o, w) \in V_+ \times V_-$, we are interested in the partition of the cycle into two flow-paths $P^{\mathrm{l}}(o, w)$ and $P^{\mathrm{r}}(o, w)$. When discussing the order of nodes along $P^{\mathrm{l}}(o, w)$, we therefore simply write $u \preccurlyeq_{\mathrm{l}} v$ instead of $u \preccurlyeq_{P^{\mathrm{l}}(o,w)} v$. We use an analogous simplification for $P^{\mathrm{r}}(o, w)$.

A first observation is that nominations can be modified such that the flow from an entry node with highest potential to an exit node with lowest potential is nonnegative, while preserving particular potential differences.

Lemma 7. *Given $\ell \in N\backslash\{0\}$ with flow $q = q(\ell)$, let $o \in V_+$ be an entry with highest potential and w a flow-meeting point with lowest potential. Furthermore, assume that $P^{\mathrm{l}}(o, w)$ and $P^{\mathrm{r}}(o, w)$ are directed paths. Then, for a given $x \in V^{\mathrm{l}}(o, w)$, a nomination $\ell' \in N$ exists such that the following properties hold (with $q' = q(\ell')$):*

$$\ell' \leq \ell, \tag{9a}$$

$$0 \leq q'_a \quad \text{for all } a \in A^{\mathrm{l}}(o, w), \tag{9b}$$

$$q'_a = q_a \quad \text{for all } a \in A^{\mathrm{r}}(o, w), \tag{9c}$$

$$\Pi_{P^{\mathrm{l}}(o,x)}(q') = \Pi_{P^{\mathrm{l}}(o,x)}(q) \geq 0, \tag{9d}$$

$$\Pi_{P^{\mathrm{l}}(o,w)}(q') = \Pi_{P^{\mathrm{l}}(o,w)}(q). \tag{9e}$$

Proof. We modify nomination ℓ and $q(\ell)$ such that the required properties are satisfied. To this end, we consider a flow decomposition as in Lemma 2.

Since $o \in V_+$ has highest potential and $P^{\mathrm{l}}(o, w)$ and $P^{\mathrm{r}}(o, w)$ are directed paths, it follows that $q_a \geq 0$ for all $a \in \delta^{\mathrm{out}}(o)$. In analogy, $q_a \geq 0$ for all $a \in \delta^{\mathrm{in}}(w)$. From Lemma 2, we then deduce that $q(P(u, v)) = 0$ if one of the following four conditions holds:

- $u \in V_+^{\mathrm{l}}(o, w)\backslash\{o\}$ and $v \in V_-^{\mathrm{r}}(o, w)\backslash\{w\}$,
- $u \in V_+^{\mathrm{r}}(o, w)\backslash\{o\}$ and $v \in V_-^{\mathrm{l}}(o, w)\backslash\{w\}$,
- $u \in V_+^{\mathrm{l}}(o, w)\backslash\{o\}$, $v \in V_-^{\mathrm{l}}(o, w)\backslash\{w\}$, and $P^{\mathrm{r}}(o, w) \subseteq P(u, v)$, or
- $u \in V_+^{\mathrm{r}}(o, w)\backslash\{o\}$, $v \in V_-^{\mathrm{r}}(o, w)\backslash\{w\}$, and $P^{\mathrm{l}}(o, w) \subseteq P(u, v)$.

In other words, since there is no flow through o or w, there cannot be a flow-path with nonzero flow through them, either. Consequently, for an arc $a \in P^{\mathrm{l}}(o, w)$, we can simplify Equation (5) to

$$q_a = \sum_{P \in \mathcal{P}_\ell^{\mathrm{l}}} \chi_a(P)\, q(P), \tag{10}$$

where $\mathcal{P}_\ell^{\mathrm{l}}$ contains all flow-paths on the left side of the cycle, i.e.,

$$\mathcal{P}_\ell^{\mathrm{l}} := \{P(u, v) \in \mathcal{P}_\ell \,:\, P(u, v) \subseteq P^{\mathrm{l}}(o, w)\}.$$

We note that $\mathcal{P}^{\mathrm{l}}_{\ell}$ depends on the choice of o and w. However, these are fixed nodes throughout this section. We now modify the flow q such that Property (9b) is satisfied. To this end, for every arc $a \in P^{\mathrm{l}}(o,w)$ and for every $P \in \mathcal{P}^{\mathrm{l}}_{\ell}$, we set the flow $q(P)=0$ if $\chi_a(P) = -1$ holds. We denote the modified flow and the corresponding nomination by q' and ℓ'. Then, for $a \in A^{\mathrm{l}}(o,w)$, the modified flow is given by

$$q'_a = \sum_{P \in \mathcal{P}^{\mathrm{l}}_{\ell} : \chi_a(P)=1} q(P) \tag{11}$$

and satisfies (9b). Furthermore, by Corollary 3, the corresponding modified nomination ℓ' satisfies (9a). Additionally, (9c) is satisfied because we have not modified any arc flows q_a for $a \in A^{\mathrm{r}}(o,w)$. Due to Lemma 4(b), the modifications possibly increase the potential difference between o and x, as well as, between o and w. This is the case if and only if the corresponding flow-path contains an arc with negative flow in q, which is now set to zero in the modified flow q'. Next, we need to iteratively adapt nomination ℓ' and flow q' to ensure the remaining properties (9d) and (9e).

Step 1: If an arc $a \in A^{\mathrm{l}}(o,x)$ with $q_a < 0$ exists, then, the potential difference between o and x is increased, i.e., $\Pi_{P^{\mathrm{l}}(o,x)}(q') > \Pi_{P^{\mathrm{l}}(o,x)}(q)$ holds. Let $u \in V^{\mathrm{l}}(o,x)$, possibly with $u=x$, be such that $q_{a'} \geq 0$ holds for all $a' \in A^{\mathrm{l}}(u,x)$ and $|V^{\mathrm{l}}(u,x)|$ is maximal. Given the flow decomposition, we then know that we have not modified arc flows on $P^{\mathrm{l}}(u,x)$. Consequently, $\Pi_{P^{\mathrm{l}}(u,x)}(q') = \Pi_{P^{\mathrm{l}}(u,x)}(q)$ holds. Thus, $\Pi_{P^{\mathrm{l}}(o,u)}(q') > \Pi_{P^{\mathrm{l}}(o,u)}(q)$ must hold. In particular, we have $a \in A^{\mathrm{l}}(o,u)$. From Lemma 2 and the construction of u it follows that for $v_1 \in V^{\mathrm{l}}_{+}(o,u)\setminus\{u\}$ and $v_2 \in V^{\mathrm{l}}_{-}(u,w)$, we have $q(P^{\mathrm{l}}(v_1,v_2))=0$. Consequently, the potential difference $\Pi_{P^{\mathrm{l}}(o,u)}(q')$ is only determined by positive path flows $q(P^{\mathrm{l}}(v_1,v_2))$ with $o \preccurlyeq_{\mathrm{l}} v_1 \preccurlyeq_{\mathrm{l}} v_2 \preccurlyeq_{\mathrm{l}} u$. We further note that $\Pi_{P^{\mathrm{l}}(o,u)}(0) = 0$ and, by Lemma 4(e), $\Pi_{P^{\mathrm{l}}(o,u)}(q) \geq 0$ holds because $\pi_o \geq \pi_u$. Consequently, due to Lemma 4(a) and (b), we can decrease path flows $q(P^{\mathrm{l}}(v_1,v_2))$ with $o \preccurlyeq_{\mathrm{l}} v_1 \preccurlyeq_{\mathrm{l}} v_2 \preccurlyeq_{\mathrm{l}} u$ to yield flow q' such that $\Pi_{P^{\mathrm{l}}(o,u)}(q') = \Pi_{P^{\mathrm{l}}(o,u)}(q)$ holds. These flow modifications only decrease the nomination at entries and exits in $V^{\mathrm{l}}(o,u)$. Thus, Lemma 4(d) implies the Properties (9a)–(9d). We note that we have not changed an arc flow of $A^{\mathrm{l}}(x,w)$ in the modifications of Step 1.

Now it is left to show that we can modify the flow q' and the corresponding nomination ℓ' such that, additionally, Property (9e) is satisfied. To this end, we assume that an arc $a \in A^{\mathrm{l}}(x,w)$ with $q_a < 0$ exists. Otherwise the claim follows directly from Lemma 4.

Step 2: If an arc $a \in A^{\mathrm{l}}(x,w)$ with $q_a < 0$ exists, then, $\Pi_{P^{\mathrm{l}}(x,w)}(q') > \Pi_{P^{\mathrm{l}}(x,w)}(q)$ holds. Let $u \in V^{\mathrm{l}}(x,w)$ be a node such that $q_{a'} \geq 0$ holds for all $a' \in A^{\mathrm{l}}(x,u)$ and $|V^{\mathrm{l}}(x,u)|$ is maximal. Given the flow decomposition, we then know that we have not modified arc flows on $A^{\mathrm{l}}(x,u)$. Thus, $\Pi_{P^{\mathrm{l}}(x,u)}(q') = \Pi_{P^{\mathrm{l}}(x,u)}(q)$ and $\Pi_{P^{\mathrm{l}}(u,w)}(q') > \Pi_{P^{\mathrm{l}}(u,w)}(q)$ hold. Furthermore, $\Pi_{P^{\mathrm{l}}(u,w)}(0) = 0$ and $\Pi_{P^{\mathrm{l}}(u,w)}(q) \geq 0$ are valid. The latter is satisfied due to $\pi_w \leq \pi_u$ and Lemma 4(e). Similar to Step 1, the potential difference $\Pi_{P^{\mathrm{l}}(u,w)}(q')$ is only determined by positive path flows $q(P^{\mathrm{l}}(v_1,v_2))$ with $u \preccurlyeq_{\mathrm{l}} v_1 \preccurlyeq_{\mathrm{l}} v_2 \preccurlyeq_{\mathrm{l}} w$. Due to Lemma 4, we can again decrease path flows $q(P^{\mathrm{l}}(v_1,v_2))$ for $u \preccurlyeq_{\mathrm{l}} v_1 \preccurlyeq_{\mathrm{l}} v_2 \preccurlyeq_{\mathrm{l}} w$ such that $\Pi_{P^{\mathrm{l}}(u,w)}(q') = \Pi_{P^{\mathrm{l}}(u,w)}(q)$ holds and Property (9e) is satisfied. Furthermore, this modification does not affect any of Properties (9b)–(9d). Since we only decrease the nomination at entries and exits, Property (9a) is also satisfied.

In total, we can modify nomination ℓ and $q(\ell)$ by repeatedly applying Steps 1 and 2 such that ℓ' and the corresponding $q(\ell')$ satisfy Properties (9). ∎

The same result can be established for the symmetric situation.

Corollary 8. *Given $\ell \in N\setminus\{0\}$ with flow $q=q(\ell)$, let $o \in V_+$ be an entry with highest potential and w a flow-meeting point with lowest potential. Furthermore, assume that $P^{\mathrm{l}}(o,w)$ and $P^{\mathrm{r}}(o,w)$ are directed paths. Then, for a given $x \in V^{\mathrm{r}}(o,w)$, a nomination $\ell' \in N$ exists such that the following properties hold (with $q' = q(\ell')$):*

$$\ell' \leq \ell, \tag{12a}$$

$$0 \leq q'_a \quad \text{for all } a \in A^{\mathrm{r}}(o,w), \tag{12b}$$

$$q'_a = q_a \quad \text{for all } a \in A^{\mathrm{l}}(o,w), \tag{12c}$$

$$\Pi_{P^{\mathrm{r}}(o,x)}(q') = \Pi_{P^{\mathrm{r}}(o,x)}(q) \geq 0, \tag{12d}$$

$$\Pi_{P^{\mathrm{r}}(o,w)}(q') = \Pi_{P^{\mathrm{r}}(o,w)}(q). \tag{12e}$$

Lemma 9. *Given $\ell \in N\setminus\{0\}$ with flow $q=q(\ell)$, let $o \in V_+$ be an entry with highest potential and w a flow-meeting point with lowest potential. Furthermore, assume that $P^{\mathrm{l}}(o,w)$ and $P^{\mathrm{r}}(o,w)$ are directed paths. Then, for given $o \preccurlyeq_{\mathrm{l}} x \preccurlyeq_{\mathrm{l}} y \preccurlyeq_{\mathrm{l}} w$ with $\Pi_{P^{\mathrm{l}}(x,y)}(q) \geq 0$, a nomination $\ell' \in N$ with $q' = q(\ell')$ exists such that Properties (9a) and (9b) are satisfied and $\Pi_{P^{\mathrm{l}}(x,y)}(q') = \Pi_{P^{\mathrm{l}}(x,y)}(q) \geq 0$ holds.*

Proof. In analogy to the proof of Lemma 7, we consider a flow decomposition of Lemma 2. Furthermore, for every arc $a \in A^{\mathrm{l}}(o,w)$, we set the flow $q(P^{\mathrm{l}}(v_1,v_2))=0$ if $\chi_a(P^{\mathrm{l}}(v_1,v_2)) = -1$ holds. Consequently, the modified flow q', given as in (11), and the corresponding nomination ℓ' satisfy (9a) and (9b). By this modification, we increase the potential difference only if an arc in $P^{\mathrm{l}}(o,w)$ with negative flow in q exists.

If an arc $a \in A^{\mathrm{l}}(o,x)$ with $q_a < 0$ exists, we apply Step 1 of the proof of Lemma 7, where we do not change the flow on any arc of $P^{\mathrm{l}}(x,w)$. On the other hand, if an arc $a \in A^{\mathrm{l}}(y,w)$ with $q_a < 0$ exists, we apply Step 2, where we do not change the flow on any arc of $P^{\mathrm{l}}(o,y)$. If an arc $a \in A^{\mathrm{l}}(x,y)$ with $q_a < 0$ exists, then, $\Pi_{P^{\mathrm{l}}(x,y)}(q') > \Pi_{P^{\mathrm{l}}(x,y)}(q) \geq 0$ holds. Due to Lemma 4(a) and (b), and $\Pi_{P^{\mathrm{l}}(x,y)}(0) = 0$, we can decrease path flows $q(P^{\mathrm{l}}(v_1,v_2))$ such that $\Pi_{P^{\mathrm{l}}(x,y)}(q') = \Pi_{P^{\mathrm{l}}(x,y)}(q)$ and Properties (9a) and (9b) are still satisfied. This modification possibly decreases the potential differences $\Pi_{P^{\mathrm{l}}(o,x)}(q')$ and $\Pi_{P^{\mathrm{l}}(y,w)}(q')$. As a consequence of Lemma 4, we deduce that $\Pi_{P^{\mathrm{l}}(o,w)}(q') \leq \Pi_{P^{\mathrm{r}}(o,w)}(q')$.

If $\Pi_{P^{\mathrm{l}}(o,w)}(q') < \Pi_{P^{\mathrm{r}}(o,w)}(q')$ is satisfied, q' is not feasible. However, this can be easily fixed. Since the arc flow of any $a \in A^{\mathrm{r}}(o,w)$ stays unchanged, $\Pi_{P^{\mathrm{r}}(o,w)}(q') = \Pi_{P^{\mathrm{r}}(o,w)}(q) \geq 0$ holds as a consequence of Lemma 4(e). Since Property (9b) is satisfied for the modified flow q', we deduce that $\Pi_{P^{\mathrm{l}}(o,w)}(q') \geq 0$. It follows that $0 = \Pi_{P^{\mathrm{r}}(o,w)}(0) \leq \Pi_{P^{\mathrm{l}}(o,w)}(q') < \Pi_{P^{\mathrm{r}}(o,w)}(q')$. By Lemma 4, we can decrease $q(P^{\mathrm{r}}(v_1,v_2))$ such that $\Pi_{P^{\mathrm{l}}(o,w)}(q') = \Pi_{P^{\mathrm{r}}(o,w)}(q')$ holds. Furthermore, $\Pi_{P^{\mathrm{l}}(x,y)}(q') = \Pi_{P^{\mathrm{l}}(x,y)}(q)$ and Properties (9a) and (9b) still hold. ∎

Analogously, we derive the symmetric result.

Corollary 10. *Given $\ell \in N\backslash\{0\}$ with flow $q = q(\ell)$, let $o \in V_+$ be an entry with highest potential and w a flow-meeting point with lowest potential. Furthermore, assume that $P^{\mathrm{l}}(o,w)$ and $P^{\mathrm{r}}(o,w)$ are directed paths. Then, for given $o \preccurlyeq_{\mathrm{r}} x \preccurlyeq_{\mathrm{r}} y \preccurlyeq_{\mathrm{r}} w$ with $\Pi_{P^{\mathrm{r}}(x,y)}(q) \geq 0$, a nomination $\ell' \in N$ with $q' = q(\ell')$ exists such that Properties (12a) and (12b) are satisfied and $\Pi_{P^{\mathrm{r}}(x,y)}(q') = \Pi_{P^{\mathrm{r}}(x,y)}(q) \geq 0$ holds.*

As a final auxiliary result, we give a sufficient condition for the existence of a unique flow-meeting point.

Lemma 11. *Given $\ell \in N\backslash\{0\}$ with flow $q = q(\ell)$, let $o \in V_+$ be an entry with highest potential and let $w \in V\backslash\{o\}$ be an arbitrary node. Furthermore, assume that $P^{\mathrm{l}}(o,w)$ and $P^{\mathrm{r}}(o,w)$ are directed paths. If $q_a \geq 0$ for all $a \in A = A^{\mathrm{l}}(o,w) \cup A^{\mathrm{r}}(o,w)$, then there is a unique flow-meeting point x. Furthermore, $x \in V^{\mathrm{l}}(o,w)$ holds.*

Proof. Since $q \geq 0$, then $\pi_w \leq \pi_v$ holds for all $v \in V$. Let $x \in V^{\mathrm{l}}(o,w)$ be such that $q_a = 0$ holds for all $a \in A^{\mathrm{l}}(x,w)$ and $|V^{\mathrm{l}}(x,w)|$ is maximal. By construction of x, it is the only flow-meeting point and $x = w$ may hold. ∎

Recall that it is sufficient to solve Problem (3) for each fixed node pair $(w_1,w_2) \in V^2$ and then check Inequality (4) to decide the feasibility of a booking. We now combine the previous results to show that an optimal solution of Problem (3) with at most one flow-meeting point exists.

Theorem 12. *Let b be a booking and let $(w_1,w_2) \in V^2$ be a fixed pair of nodes. Then, there is an optimal solution of Problem (3) that has at most one flow-meeting point w.*

Proof. Let (ℓ, q, π) be an optimal solution of (3). Choose an entry $o \in V_+$ with highest potential and a flow-meeting point w with lowest potential. Due to Lemma 6, $\pi_w \leq \pi_v$ holds for all $v \in V$. Without loss of generality, we assume that $P^{\mathrm{l}}(o,w)$ and $P^{\mathrm{r}}(o,w)$ are directed.

The zero nomination corresponds to a feasible point that satisfies the claim and $\pi_{w_1} - \pi_{w_2} = 0$. Thus, we can assume that

$$\pi_{w_1} - \pi_{w_2} > 0 \tag{13}$$

holds. If there is only one flow-meeting point, we are done. Hence, we now additionally assume that ℓ admits at least two different flow-meeting points.

Case 1: $w_1 \in V^{\mathrm{l}}(o,w)$ and $w_2 \in V^{\mathrm{r}}(o,w)$ hold. Thus, we can equivalently reformulate (13) as

$$0 < \pi_{w_1} - \pi_{w_2} = -\Pi_{P^{\mathrm{l}}(o,w_1)}(q) + \Pi_{P^{\mathrm{r}}(o,w_2)}(q).$$

We now apply Lemma 7 with $x = w_1$, which does not change $\Pi_{P^{\mathrm{l}}(o,w_1)}(q)$ and $\Pi_{P^{\mathrm{r}}(o,w_2)}(q)$. Then, we apply Corollary 8 with $x = w_2$, which does not change $\Pi_{P^{\mathrm{l}}(o,w_1)}(q)$ and $\Pi_{P^{\mathrm{r}}(o,w_2)}(q)$. Consequently, the obtained nomination ℓ' and the corresponding flow $q' = q(\ell')$ are still optimal. Thus, (13) is satisfied by $q(\ell') \geq 0$. The claim then follows by Lemma 11.

Case 2: $w_1 \in V^{\mathrm{r}}(o,w)$ and $w_2 \in V^{\mathrm{l}}(o,w)$ hold. The claim follows in analogy to Case 1.

Case 3: $w_1, w_2 \in V^{\mathrm{l}}(o,w)$ and $w_1 \preccurlyeq_{\mathrm{l}} w_2$. In this case, (13) reads

$$0 < \pi_{w_1} - \pi_{w_2} = \Pi_{P^{\mathrm{l}}(w_1,w_2)}(q).$$

We first apply Corollary 8 with $x = w$, which does not change $\Pi_{P^{\mathrm{l}}(w_1,w_2)}(q)$. Thus, (13) is still satisfied and $q'_a \geq 0$ holds for every $a \in P^{\mathrm{r}}(o,w)$. We now apply Lemma 9 with $x = w_1$ and $y = w_2$, which does not change the objective value $\pi_{w_1} - \pi_{w_2} = \Pi_{P^{\mathrm{l}}(w_1,w_2)}(q)$. Consequently, $q' \geq 0$ holds and (13) is still satisfied. The claim then again follows from Lemma 11.

Case 4: $w_1, w_2 \in V^{\mathrm{r}}(o,w)$ and $w_1 \preccurlyeq_{\mathrm{r}} w_2$. The claim follows in analogy to Case 3.

Case 5: $w_1, w_2 \in V^{\mathrm{l}}(o,w)$ and $w_2 \preccurlyeq_{\mathrm{l}} w_1$. Inequality (13) then reads

$$0 < \pi_{w_1} - \pi_{w_2} = -\Pi_{P^{\mathrm{l}}(w_2,w_1)}(q).$$

We first apply Corollary 8 with $x = w$, which does not change $\Pi_{P^{\mathrm{l}}(w_2,w_1)}(q)$. Thus, (13) is still satisfied and $q'_a \geq 0$ for every $a \in P^{\mathrm{r}}(o,w)$. Now take $u \in V^{\mathrm{l}}(o,w)$ such that $q'_a \geq 0$ for all $a \in A^{\mathrm{l}}(u,w)$ and $|A^{\mathrm{l}}(u,w)|$ is maximal. If $u \in V^{\mathrm{l}}(o,w_2)$, then $q'_a \geq 0$ for all $a \in A^{\mathrm{l}}(w_2,w_1)$. Thus, $\Pi_{P^{\mathrm{l}}(w_2,w_1)}(q) \geq 0$ also holds, which contradicts (13). Hence, we conclude that $u \in V^{\mathrm{l}}(w_2,w) \setminus \{w_2\}$. By Lemma 2 and the construction of u, we deduce that for $a \in A^{\mathrm{l}}(u,w)$ the flow is given by

$$q'_a = \sum_{P \in \overline{\mathcal{P}}^{\mathrm{l}}_{\ell}} q(P), \quad \overline{\mathcal{P}}^{\mathrm{l}}_{\ell} := \{P \in \mathcal{P}_{\ell} : P \subseteq P^{\mathrm{l}}(u,w), \chi_a(P) = 1\}.$$

We now set the flow $q(P^{\mathrm{l}}) = 0$ for $P^{\mathrm{l}} \subseteq P^{\mathrm{l}}(u,w)$ and $\chi_a(P^{\mathrm{l}}) = 1$. By this modification, we have possibly decreased $\Pi_{P^{\mathrm{l}}(w_2,w_1)}$ and thus also $\Pi_{P^{\mathrm{l}}(o,w)}$. In particular, (13) is still satisfied. Lemma 4(d) implies

$$\Pi_{P^{\mathrm{l}}(o,w)}(q') = \Pi_{P^{\mathrm{l}}(o,u)}(q') + \Pi_{P^{\mathrm{l}}(u,w)}(q').$$

After modification, we have $\Pi_{P^{\mathrm{l}}(u,w)}(q') = \Pi_{P^{\mathrm{l}}(u,w)}(0) = 0$ and $\Pi_{P^{\mathrm{l}}(o,u)}(q') = \Pi_{P^{\mathrm{l}}(o,u)}(q)$. By Lemma 4(e) and $\pi_o \geq \pi_u$, $\Pi_{P^{\mathrm{l}}(o,u)}(q)$ is nonnegative. We deduce that $\Pi_{P^{\mathrm{l}}(o,u)}(q') \geq 0$. Given Lemma 4(a) and (b), we can now decrease path flows $q(P^{\mathrm{r}})$ such that $\Pi_{P^{\mathrm{l}}(o,w)}(q') = \Pi_{P^{\mathrm{r}}(o,w)}(q')$ holds. After this modification, (13) is still satisfied and its value is possibly increased, i.e., the objective function value $\pi_{w_1} - \pi_{w_2}$ is possibly increased by the modifications. Consequently, the obtained solution is still optimal. Moreover, w is now connected to a flow-meeting point in $V^{\mathrm{l}}(o,u)$ because $q'_a = 0$ holds for all $a \in P^{\mathrm{l}}(u,w)$. Consequently, for nomination ℓ' a flow-meeting point in $V^{\mathrm{l}}(o,u)$ with lowest potential exists. We now repeat this procedure until either the claim holds or a new flow-meeting point with lowest potential is an element of $V^{\mathrm{l}}(o,w_1)$. Then, we apply the respective case of Cases 1–4.

Case 6: $w_1, w_2 \in V^{\mathrm{r}}(o,w)$ and $w_2 \preccurlyeq_{\mathrm{r}} w_1$. The claim follows in analogy to Case 5. ∎

As a direct consequence of this result, we deduce the following corollary.

Corollary 13. *Let b be a booking and let $(w_1,w_2) \in V^2$ be a fixed pair of nodes. Then, there exist nodes $(o,w) \in V_+ \times V_-$ and an optimal solution (ℓ,q,π) of Problem (3) with $q \geq 0$, if we assume that $P^{\mathrm{l}}(o,w)$ and $P^{\mathrm{r}}(o,w)$ are directed paths.*

The previous result implies that when determining potential-difference maximizing nominations solving Problem (3) for fixed $(w_1,w_2) \in V^2$, we can additionally restrict the search space by iteratively considering $(o,w) \in V_+ \times V_-$ and imposing that there is flow from o to w. This is further formalized and exploited in the next section.

5 | STRUCTURE OF POTENTIAL-DIFFERENCE MAXIMIZING NOMINATIONS

In this section, we fix $(w_1,w_2) \in V^2$ and show that there exist optimal solutions of (3) with additional structure that allows us to reduce the dimension of the problem. Based on the results of Section 5, in particular, Corollary 13, we next show that (4) can be decided by considering the following variant of Problem (3) for every $(o,w) \in V_+ \times V_-$:

$$\begin{aligned}
\overline{\varphi}^{ow}_{w_1w_2}(b) := \max_{\ell,q,\pi} \quad & \pi_{w_1} - \pi_{w_2} && \text{(14a)}\\
\text{s.t.} \quad & \sum_{a \in \delta^{\mathrm{out}}(u)} q_a - \sum_{a \in \delta^{\mathrm{in}}(u)} q_a = \sigma_u \ell_u, \quad u \in V, &&\\
& 0 \leq \ell_u \leq b_u, \quad u \in V, &&\\
& \pi_u - \pi_v = \Lambda_a q_a |q_a|, \quad a \in A', && \text{(14b)}\\
& q_a \geq 0, \quad a \in A', && \text{(14c)}
\end{aligned}$$

where b is a booking and A' is obtained from A by orienting all arcs from o to w. Note that in addition to the constraints of (3), we now also impose nonnegative flow from o to w, thus effectively reducing the feasible domain of the problem.

Theorem 14. *Let b be a booking. Then*

$$\varphi_{w_1 w_2}(b) = \max_{(o,w)\in V_+\times V_-} \overline{\varphi}^{ow}_{w_1 w_2}(b)$$

holds. Furthermore, the optimal values are finite and attained.

Proof. First, observe that ℓ is bounded in (3). As a consequence of Theorem 7.1 of Chapter 7 in [24], an optimal solution of (3) with finite optimal value exists, i.e., $\varphi_{w_1 w_2}(b) < \infty$.

Let (ℓ, q, π) be an optimal solution corresponding to $\max_{(o,w)\in V_+\times V_-} \overline{\varphi}^{ow}_{w_1 w_2}(b)$. First, observe that the arc orientation does not play any role in Problem (3). If an arc has a different orientation, we just switch the sign of the corresponding flow variable. Thus, we assume w.l.o.g. that $P^{\mathrm{l}}(o,w)$ and $P^{\mathrm{r}}(o,w)$ are directed paths in the given instance of (3). Consequently, (ℓ, q, π) is feasible for (3). Thus,

$$\varphi_{w_1 w_2}(b) \geq \max_{(o,w)\in V_+\times V_-} \overline{\varphi}^{ow}_{w_1 w_2}(b).$$

The other inequality follows directly from Corollary 13. ∎

As a consequence, the feasibility of a booking can be characterized using Problem (14) as follows.

Corollary 15. *A booking b is feasible if and only if for every pair $(w_1, w_2) \in V^2$ and for every $(o,w) \in V_+ \times V_-$,*

$$\overline{\varphi}^{ow}_{w_1 w_2}(b) \leq \pi^+_{w_1} - \pi^-_{w_2}. \tag{15}$$

We now further analyze the structure of optimal solutions of (14) for fixed $(o,w) \in V_+ \times V_-$ and given $(w_1, w_2) \in V^2$ w.r.t. their respective position in the cycle. Without loss of generality, we assume that $P^{\mathrm{l}}(o,w)$ and $P^{\mathrm{r}}(o,w)$ are directed paths.

5.1 | Nodes on different sides of *G*

Assume that $w_1 \in P^{\mathrm{l}}(o,w)$ and $w_2 \in P^{\mathrm{r}}(o,w)$ hold. We show that an optimal solution (ℓ, q, π) of (14) exists that additionally satisfies the following properties:

(a) Two entries $s^l_1, s^l_2 \in V^{\mathrm{l}}_+(o,w)$ with $s^l_1 \preccurlyeq_{\mathrm{l}} s^l_2$ exist such that

$$\ell_v = 0, \quad v \in (V^{\mathrm{l}}_+(o, s^l_1) \cup V^{\mathrm{l}}_+(s^l_2, w)) \backslash \{o, s^l_1, s^l_2\},$$
$$\ell_v = b_v, \quad v \in V^{\mathrm{l}}_+(s^l_1, s^l_2) \backslash \{s^l_1, s^l_2\}.$$

(b) An exit $t^l_1 \in V^{\mathrm{l}}_-(o,w)$ exists such that

$$\ell_v = 0, \quad v \in V^{\mathrm{l}}_-(o, t^l_1) \backslash \{t^l_1\},$$
$$\ell_v = b_v, \quad v \in V^{\mathrm{l}}_-(t^l_1, w) \backslash \{t^l_1\}.$$

(c) An entry $s^r_1 \in V^{\mathrm{r}}_+(o,w)$ exists such that

$$\ell_v = b_v, \quad v \in V^{\mathrm{r}}_+(o, s^r_1) \backslash \{s^r_1\},$$
$$\ell_v = 0, \quad v \in V^{\mathrm{r}}_+(s^r_1, w) \backslash \{s^r_1\}.$$

(d) Two exits $t^r_1, t^r_2 \in V^{\mathrm{r}}_-(o,w)$ with $t^r_1 \preccurlyeq_{\mathrm{r}} t^r_2$ exist such that

$$\ell_v = 0, \quad v \in (V^{\mathrm{r}}_-(o, t^r_1) \cup V^{\mathrm{r}}_-(t^r_2, w)) \backslash \{t^r_1, t^r_2, w\},$$
$$\ell_v = b_v, \quad v \in V^{\mathrm{r}}_-(t^r_1, t^r_2) \backslash \{t^r_1, t^r_2\}.$$

A possible configuration of nodes $o, w_1, s^l_1, s^l_2, t^l_1, w, w_2, s^r_1, t^r_1, t^r_2$ is given in Figure 3. To show the existence of such a solution, we introduce a bilevel problem, where the lower level is given by (14) and the upper level chooses, among all lower-level optimal solutions, one with the additional structure. It is given by

$$\min_{x,y} \quad f_1(\ell, x^{\leqslant_{\mathrm{l}}}, x^{\geqslant_{\mathrm{l}}}) + f_2(\ell, y^{\leqslant_{\mathrm{l}}}) + f_3(\ell, x^{\geqslant_{\mathrm{r}}}) + f_4(\ell, y^{\leqslant_{\mathrm{r}}}, y^{\geqslant_{\mathrm{r}}}) \tag{16a}$$

$$\text{s.t.} \quad (\ell, q, \pi) \text{ solves } (14),$$

$$Mx_v^{\leqslant_{\mathrm{l}}} \geq \sum_{u \in V_+^{\mathrm{l}}(o,v)\setminus\{o\}} \ell_u, \quad v \in V_+^{\mathrm{l}}(o,w)\setminus\{o\}, \tag{16b}$$

$$Mx_v^{\geqslant_{\mathrm{l}}} \geq \sum_{u \in V_+^{\mathrm{l}}(v,w)} \ell_u, \quad v \in V_+^{\mathrm{l}}(o,w)\setminus\{o\}, \tag{16c}$$

$$My_v^{\leqslant_{\mathrm{l}}} \geq \sum_{u \in V_-^{\mathrm{l}}(o,v)} \ell_u, \quad v \in V_-^{\mathrm{l}}(o,w), \tag{16e}$$

$$Mx_v^{\geqslant_{\mathrm{r}}} \geq \sum_{u \in V_+^{\mathrm{r}}(v,w)} \ell_u, \quad v \in V_+^{\mathrm{r}}(o,w), \tag{16e}$$

$$My_v^{\leqslant_{\mathrm{r}}} \geq \sum_{u \in V_-^{\mathrm{r}}(o,v)} \ell_u, \quad v \in V_-^{\mathrm{r}}(o,w)\setminus\{w\}, \tag{16f}$$

$$My_v^{\geqslant_{\mathrm{r}}} \geq \sum_{u \in V_-^{\mathrm{r}}(v,w)\setminus\{w\}} \ell_u, \quad v \in V_-^{\mathrm{r}}(o,w)\setminus\{w\}, \tag{16g}$$

$$x_v^{\leqslant_{\mathrm{l}}}, x_v^{\geqslant_{\mathrm{l}}}, x_v^{\geqslant_{\mathrm{r}}}, y_v^{\leqslant_{\mathrm{l}}}, y_v^{\leqslant_{\mathrm{r}}}, y_v^{\geqslant_{\mathrm{r}}} \in \{0,1\}, \quad v \in V, \tag{16h}$$

where $M = \sum_{u \in V} b_u$ and $f_1, \ldots, f_4$ are continuous functions that we specify later. By Constraints (16b) and (16c), the variables $x_v^{\leqslant_{\mathrm{l}}}$ and $x_v^{\geqslant_{\mathrm{l}}}$ model the existence of an active entry before and after v on P^{l}. Similarly, Constraints (16d) ensure that $y_v^{\leqslant_{\mathrm{l}}}$ determines the existence of an active exit before v on P^{l}. An analogous interpretation can be given for Constraints (16e)–(16g) and the variables $x^{\geqslant_{\mathrm{r}}}$, $y^{\leqslant_{\mathrm{r}}}$, $y^{\geqslant_{\mathrm{r}}}$. Then, the optimal value function reformulation of (16) is given by

$$\min_{\ell,q,\pi,x,y} \quad f_1(\ell, x^{\leqslant_{\mathrm{l}}}, x^{\geqslant_{\mathrm{l}}}) + f_2(\ell, y^{\leqslant_{\mathrm{l}}}) + f_3(\ell, x^{\geqslant_{\mathrm{r}}}) + f_4(\ell, y^{\leqslant_{\mathrm{r}}}, y^{\geqslant_{\mathrm{r}}}) \tag{17a}$$

$$\text{s.t.} \quad (1a), (3b), (14b), (14c), \tag{17b}$$

$$(16b)\text{–}(16h), \tag{17c}$$

$$\pi_{w_1} - \pi_{w_2} \geq \overline{\varphi}_{w_1 w_2}^{ow}(b). \tag{17d}$$

Here, Constraint (17b) determines the feasible domain of Problem (14) and Constraint (17d) guarantees feasible points with a potential difference of at least $\overline{\varphi}_{w_1 w_2}^{ow}(b)$. Thus, we only consider optimal solutions of (14). We denote by

$$z := (\ell, q, \pi, x^{\leqslant_{\mathrm{l}}}, x^{\geqslant_{\mathrm{l}}}, x^{\geqslant_{\mathrm{r}}}, y^{\leqslant_{\mathrm{l}}}, y^{\leqslant_{\mathrm{r}}}, y^{\geqslant_{\mathrm{r}}})$$

a feasible point of (17). In particular, we have the following result.

Lemma 16. *Let z be feasible for (17). Then (ℓ, q, π) is an optimal solution of (14). Conversely, every optimal solution of (14) can be extended to a feasible point of (17).*

Proof. The first statement follows from the previous discussion. For the converse, let an optimal solution (ℓ, q, π) of (14) be given. We construct a solution z as follows:

$$x_v^{\leqslant_{\mathrm{l}}} = 1, \quad \text{if and only if an active } u \in V_+^{\mathrm{l}}(o,v)\setminus\{o\} \text{ exists},$$

$$x_v^{\geqslant_{\mathrm{l}}} = 1, \quad \text{if and only if an active } u \in V_+^{\mathrm{l}}(v,w)\setminus\{o\} \text{ exists},$$

$$y_v^{\leqslant_{\mathrm{l}}} = 1, \quad \text{if and only if an active } u \in V_-^{\mathrm{l}}(o,v) \text{ exists},$$

$$x_v^{\geqslant_{\mathrm{r}}} = 1, \quad \text{if and only if an active } u \in V_+^{\mathrm{r}}(v,w) \text{ exists},$$

$$y_v^{\leqslant_{\mathrm{r}}} = 1, \quad \text{if and only if an active } u \in V_-^{\mathrm{r}}(o,v)\setminus\{w\} \text{ exists},$$

$$y_v^{\geqslant_{\mathrm{r}}} = 1, \quad \text{if and only if an active } u \in V_-^{\mathrm{r}}(v,w)\setminus\{w\} \text{ exists}.$$

■

We now specify the parts of the objective function of (17) and prove connections between these functions and the stated Properties (a)–(d). We discuss and prove the results for f_1 and f_2 in detail, whereas we only state the results for f_3 and f_4, since they are very similar. The proofs for the results concerning f_3 and f_4 can be found in Appendix A.

For the following proofs, we make use of structures resulting from the negation of Properties (a)–(d) on Page 11. More precisely, we observe that

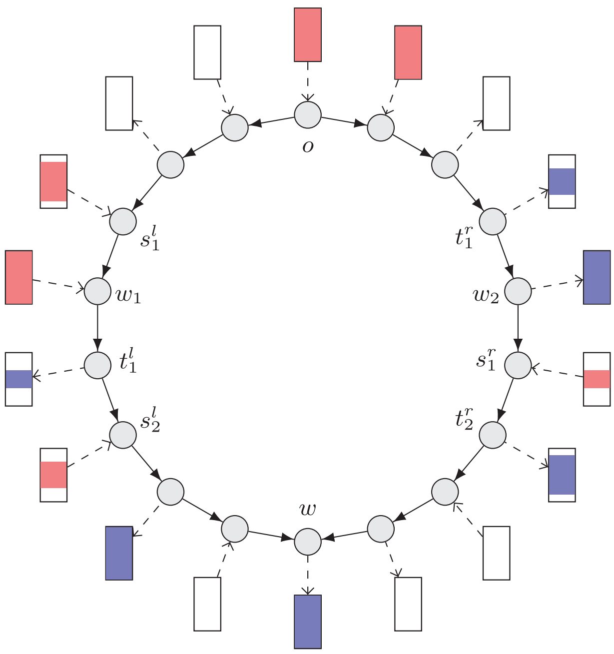

FIGURE 3 Configuration of s and t nodes if $w_1 \in P^{\mathrm{l}}(o,w)$ and $w_2 \in P^{\mathrm{r}}(o,w)$. Boxes qualitatively illustrate the amount of the booking that is nominated

- if Property (a) does not hold, then there are $u_1, u_2, u_3 \in V^{\mathrm{l}}_{+}(o,w)\setminus\{o\}$ with $u_1 \prec_{\mathrm{l}} u_2 \prec_{\mathrm{l}} u_3$ such that $\ell_{u_1} > 0, \ell_{u_2} < b_{u_2}$, and $\ell_{u_3} > 0$,
- if Property (b) does not hold, then there are $u_1, u_2 \in V^{\mathrm{l}}_{-}(o,w)$ with $u_1 \prec_{\mathrm{l}} u_2$ such that $\ell_{u_1} > 0$ and $\ell_{u_2} < b_{u_2}$,
- if Property (c) does not hold, then there are $u_1, u_2 \in V^{\mathrm{r}}_{+}(o,w)$ with $u_1 \prec_{\mathrm{l}} u_2$ such that $\ell_{u_1} < b_{u_1}$ and $\ell_{u_2} > 0$, and
- if Property (d) does not hold, then there are $u_1, u_2, u_3 \in V^{\mathrm{r}}_{-}(o,w)\setminus\{o\}$ with $u_1 \prec_{\mathrm{l}} u_2 \prec_{\mathrm{l}} u_3$ such that $\ell_{u_1} > 0, \ell_{u_2} < b_{u_2}$, and $\ell_{u_3} > 0$.

Consider, for instance, the negation of Property (a). It is always possible to satisfy the first part of the property, i.e., there exist two entries $s_1^l, s_2^l \in V^{\mathrm{l}}_{+}(o,w)$ with $s_1^l \preccurlyeq_{\mathrm{l}} s_2^l$ such that

$$\ell_v = 0, \quad v \in (V^{\mathrm{l}}_{+}(o,s_1^l) \cup V^{\mathrm{l}}_{+}(s_2^l,w))\setminus\{o, s_1^l, s_2^l\}.$$

To achieve this, we simply choose the first and the last active entry node on the left side of the cycle, i.e., $s_1^l \preccurlyeq_{\mathrm{l}} s_2^l \in V^{\mathrm{l}}_{+}(o,w)$ such that $\ell_{s_1^l} > 0, \ell_{s_2^l} > 0$, and $\ell_u = 0$ for all $u \in V^{\mathrm{l}}_{+}(o,s_1^l) \cup V^{\mathrm{l}}_{+}(s_2^l,w)\setminus\{o, s_1^l, s_2^l\}$. Now, if Property (a) is not satisfied, there has to exist another node $u \in V^{\mathrm{l}}_{+}(s_1^l,s_2^l)\setminus\{s_1^l, s_2^l\}$ with $\ell_u < b_u$, which shows the claim. Analogously, we can obtain the remaining statements.

Lemma 17. *Let z be feasible for (17) and*

$$f_1(\ell, x^{\preccurlyeq_{\mathrm{l}}}, x^{\succcurlyeq_{\mathrm{l}}}) := \sum_{\substack{i,j \in V^{\mathrm{l}}_{+}(o,w)\setminus\{o\}: \\ i \preccurlyeq_{\mathrm{l}} j}} x_i^{\preccurlyeq_{\mathrm{l}}} x_j^{\succcurlyeq_{\mathrm{l}}} \sum_{v \in V^{\mathrm{l}}_{+}(i,j)\setminus\{i,j\}} (b_v - \ell_v). \tag{18}$$

Then, there exists $(x^{\preccurlyeq_{\mathrm{l}}}, x^{\succcurlyeq_{\mathrm{l}}})$ such that $f_1(\ell, x^{\preccurlyeq_{\mathrm{l}}}, x^{\succcurlyeq_{\mathrm{l}}}) = 0$ holds if and only if ℓ satisfies Property (a).

Proof. Let z be feasible for (17). For $i,j \in V^{\mathrm{l}}_{+}(o,w)\setminus\{o\}$ where $i \preccurlyeq_{\mathrm{l}} j$,

$$x_i^{\preccurlyeq_{\mathrm{l}}} x_j^{\succcurlyeq_{\mathrm{l}}} \sum_{v \in V^{\mathrm{l}}_{+}(i,j)\setminus\{i,j\}} (b_v - \ell_v) \geq 0$$

holds. Assume now that Property (a) does not hold. Consequently, there are $u_1, u_2, u_3 \in V^{\mathrm{l}}_{+}(o,w)\setminus\{o\}$ with $u_1 \prec_{\mathrm{l}} u_2 \prec_{\mathrm{l}} u_3$ such that $\ell_{u_1} > 0, \ell_{u_2} < b_{u_2}$, and $\ell_{u_3} > 0$ hold. Thus, $x_{u_1}^{\preccurlyeq_{\mathrm{l}}} = 1 = x_{u_3}^{\succcurlyeq_{\mathrm{l}}}$ and $\sum_{v \in V^{\mathrm{l}}_{+}(u_1,u_3)\setminus\{u_1,u_3\}} (b_v - \ell_v) > 0$, therefore

$$x_{u_1}^{\preccurlyeq_{\mathrm{l}}} x_{u_3}^{\succcurlyeq_{\mathrm{l}}} \sum_{v \in V^{\mathrm{l}}_{+}(u_1,u_3)\setminus\{u_1,u_3\}} (b_v - \ell_v) > 0$$

holds. Consequently, $f_1(\ell, x^{\preccurlyeq_{\mathrm{l}}}, x^{\succcurlyeq_{\mathrm{l}}}) > 0$.

If ℓ satisfies Property (a), then we set $x_u^{\preccurlyeq_l} = 0$ for all $u \in P^l(o, s_1^l)\setminus\{s_1^l\}$. Otherwise, we set $x_u^{\preccurlyeq_l} = 1$. Additionally, we set $x_u^{\succcurlyeq_l} = 1$ for all $u \in P^l(o, s_2^l)$ and otherwise we set $x_u^{\succcurlyeq_l} = 0$. Consequently, for $i \in V_+^l(o, s_1^l)\setminus\{s_1^l\}$ or $j \in V_+^l(s_2^l, w)\setminus\{s_2^l\}$, we have $x_i^{\preccurlyeq_l} x_j^{\succcurlyeq_l} = 0$ and for $i,j \in V_+^l(s_1^l, s_2^l)$,

$$\sum_{v \in V_+^l(i,j)\setminus\{i,j\}} (b_v - \ell_v) = 0$$

holds due to Property (a). Consequently, $f_1(\ell, x^{\preccurlyeq_l}, x^{\succcurlyeq_l}) = 0$ holds. ∎

Lemma 18. *Let z be feasible for (17) and*

$$f_2(\ell, y^{\preccurlyeq_l}) := \sum_{i \in V_-^l(o,w)} y_i^{\preccurlyeq_l} \sum_{v \in V_-^l(i,w)\setminus\{i\}} (b_v - \ell_v). \tag{19}$$

Then, there exists $y^{\preccurlyeq_l}$ such that $f_2(\ell, y^{\preccurlyeq_l}) = 0$ holds if and only if ℓ satisfies Property (b).

Proof. Let z be feasible for (17). For $i \in V_-^l(o, w)$,

$$y_i^{\preccurlyeq_l} \sum_{v \in V_-^l(i,w)\setminus\{i\}} (b_v - \ell_v) \geq 0$$

holds. Assume now that Property (b) does not hold. Consequently, there are $u_1, u_2 \in V_-^l(o, w)$ with $u_1 \prec_l u_2$ such that $\ell_{u_1} > 0$ and $\ell_{u_2} < b_{u_2}$ hold. Thus, $y_{u_1}^{\preccurlyeq_l} = 1$ and

$$\sum_{v \in V_-^l(u_1,w)\setminus\{u_1\}} (b_v - \ell_v) > 0$$

holds, which implies $f_2(\ell, y^{\preccurlyeq_l}) > 0$.

If ℓ satisfies Property (b), then we set $y_u^{\preccurlyeq_l} = 0$ for all $u \in V_-^l(o, t_1^l)\setminus\{t_1^l\}$. Otherwise, we set $y_u^{\preccurlyeq_l} = 1$. Furthermore, for $i \in V_-^l(t_1^l, w)$,

$$\sum_{v \in V_-^l(i,w)\setminus\{i\}} (b_v - \ell_v) = 0$$

holds due to Property (b). Consequently, $f_2(\ell, y^{\preccurlyeq_l}) = 0$ holds. ∎

Lemma 19. *Let z be feasible for (17) and*

$$f_3(\ell, x^{\succcurlyeq_r}) := \sum_{i \in V_+^r(o,w)} x_i^{\succcurlyeq_r} \sum_{v \in V_+^r(o,i)\setminus\{i\}} (b_v - \ell_v). \tag{20}$$

Then, there exists $x^{\succcurlyeq_r}$ such that $f_3(\ell, x^{\succcurlyeq_r}) = 0$ holds if and only if ℓ satisfies Property (c).

Lemma 20. *Let z be feasible for (17) and*

$$f_4(\ell, y^{\preccurlyeq_r}, y^{\succcurlyeq_r}) = \sum_{\substack{i,j \in V_-^r(o,w)\setminus\{w\}: \\ i \preccurlyeq_r j}} y_i^{\preccurlyeq_r} y_j^{\succcurlyeq_r} \sum_{v \in V_-^r(i,j)\setminus\{i,j\}} (b_v - \ell_v). \tag{21}$$

Then, there exists $(y^{\preccurlyeq_r}, y^{\succcurlyeq_r})$ such that $f_4(\ell, y^{\preccurlyeq_r}, y^{\succcurlyeq_r}) = 0$ holds if and only if ℓ satisfies Property (d).

In the following, we consider $f_1, \dots, f_4$ as specified in Lemmas 17–20. As a next step, we show that changing the nomination ℓ on the boundary nodes of Properties (a)–(d) does not affect the values of $f_1, \dots, f_4$, since the corresponding products of binary variables are zero.

Lemma 21. *Let z be an optimal solution of (17) and let $u_1, u_3 \in V_+^l(o, w)$ with $u_1 \preccurlyeq_l u_3$ be nodes such that $\ell_{u_1} > 0$, $\ell_{u_3} > 0$, $\ell_u = 0$ for all $u \in (V_+^l(o, u_1) \cup V_+^l(u_3, w))\setminus\{o, u_1, u_3\}$. Suppose further that z' is feasible for (17) with*

$$\ell'_{u_1} > 0, \quad \ell'_{u_3} > 0, \quad \ell'_u = \ell_u, \quad u \in V_+^l(o, w)\setminus\{o, u_1, u_3\}.$$

Then, $f_1(\ell', x^{\preccurlyeq_l}, x^{\succcurlyeq_l}) = f_1(\ell, x^{\preccurlyeq_l}, x^{\succcurlyeq_l})$ holds.

Proof. Optimality of z and the choice of u_1 and u_3 imply $x_u^{\preccurlyeq_l} = 0$ for all $u \in V_+^l(o, u_1)\setminus\{o, u_1\}$ and $x_u^{\succcurlyeq_l} = 0$ for all $u \in V_+^l(u_3, w)\setminus\{u_3\}$. Hence, for $i,j \in V_+^l(o, w)\setminus\{o\}$ with $i \preccurlyeq_l j$ we have

$$x_i^{\preccurlyeq_l} x_j^{\succcurlyeq_l} \sum_{v \in V_+^l(i,j)\setminus\{i,j\}} (b_v - \ell_v) = 0,$$

whenever u_1 or u_3 is in $V_+^{\mathrm{l}}(i,j)\setminus\{i,j\}$, because then $x_i^{\preccurlyeq_\mathrm{l}} x_j^{\succcurlyeq_\mathrm{l}} = 0$. Consequently, a change of ℓ_{u_1} or ℓ_{u_3} does not change $f_1(\ell, x^{\preccurlyeq_\mathrm{l}}, x^{\succcurlyeq_\mathrm{l}})$. ■

Lemma 22. *Let z be an optimal solution of (17) and let $v_1 \in V_-^{\mathrm{l}}(o,w)$ be a node such that $\ell_{v_1} > 0$ and $\ell_v = 0$ for all $v \in V_-^{\mathrm{l}}(o,v_1)\setminus\{v_1\}$. Suppose further that z' is feasible for (17) with*

$$\ell'_{v_1} > 0, \quad \ell'_v = \ell_v, \quad u \in V_-^{\mathrm{l}}(o,w)\setminus\{v_1, w\}.$$

Then, $f_2(\ell', y^{\preccurlyeq_\mathrm{l}}) = f_2(\ell, y^{\preccurlyeq_\mathrm{l}})$ holds.

Proof. Optimality of z and the choice of v_1 imply $y_v^{\preccurlyeq_\mathrm{l}} = 0$ for all $v \in V_-^{\mathrm{l}}(o,v_1)\setminus\{v_1\}$. Hence,

$$y_i^{\preccurlyeq_\mathrm{l}} \sum_{v \in V_-^{\mathrm{l}}(i,w)\setminus\{i\}} (b_v - \ell_v) = 0$$

holds whenever $v_1 \in V_-^{\mathrm{l}}(i,w)\setminus\{i\}$. Thus, a change of ℓ_{v_1} does not change $f_2(\ell, y^{\preccurlyeq_\mathrm{l}})$. ■

Lemma 23. *Let z be an optimal solution of (17) and let $u_1 \in V_+^{\mathrm{r}}(o,w)$ be a node such that $\ell_{u_1} > 0$ and $\ell_u = 0$ for all $u \in V_+^{\mathrm{r}}(u_1,w)\setminus\{u_1\}$. Suppose further that z' is feasible for (17) with*

$$\ell'_{u_1} > 0, \quad \ell'_u = \ell_u, \quad u \in V_+^{\mathrm{r}}(o,w)\setminus\{o, u_1\}.$$

Then, $f_3(\ell, x^{\succcurlyeq_\mathrm{r}}) = f_3(\tilde{\ell}, x^{\succcurlyeq_\mathrm{r}})$ holds.

Lemma 24. *Let z be an optimal solution of (17) and let $v_1, v_3 \in V_-^{\mathrm{r}}(o,w)$ with $v_1 \preccurlyeq_\mathrm{r} v_3$ be nodes such that $\ell_{v_1} > 0$, $\ell_{v_3} > 0$, $\ell_u = 0$ for all $u \in (V_-^{\mathrm{r}}(o,v_1) \cup V_-^{\mathrm{r}}(v_3,w))\setminus\{v_1, v_3, w\}$. Suppose further that z' is feasible for (17) with*

$$\ell'_{v_1} > 0, \quad \ell'_{v_3} > 0, \quad \ell'_u = \ell_u, \quad u \in V_-^{\mathrm{r}}(o,w)\setminus\{v_1, v_3, w\}.$$

Then, $f_4(\ell', y^{\preccurlyeq_\mathrm{r}}, y^{\succcurlyeq_\mathrm{r}}) = f_4(\ell, y^{\preccurlyeq_\mathrm{r}}, y^{\succcurlyeq_\mathrm{r}})$ holds.

The two last proofs can again be found in Appendix A. We next show that there is an optimal solution of (14) that satisfies Properties (a)–(d). More precisely, we prove that the optimal value of (17) is zero by individually treating $f_1, \dots, f_4$. The final result then easily follows from Lemmas 17–20.

Lemma 25. *If z is an optimal solution of (17), then $f_1(\ell, x^{\preccurlyeq_\mathrm{l}}, x^{\succcurlyeq_\mathrm{l}}) = 0$ holds.*

Proof. Let z be an optimal solution of (17). By contradiction, we assume that $f_1(\ell, x^{\preccurlyeq_\mathrm{l}}, x^{\succcurlyeq_\mathrm{l}}) > 0$ holds. Lemma 17 implies that ℓ does not satisfy Property (a). Consequently, there are entries $u_1, u_2, u_3 \in V_+^{\mathrm{l}}(o,w)\setminus\{o\}$ with $u_1 \prec_\mathrm{l} u_2 \prec_\mathrm{l} u_3$ such that $\ell_{u_1} > 0, \ell_{u_2} < b_{u_2}$, and $\ell_{u_3} > 0$. If $q_a > 0$ for $a \in \delta^{\mathrm{out}}(o) \cap P^{\mathrm{l}}(o,w)$, we replace $u_1 = o$. Otherwise, we choose $u_1 \neq o$ such that $\ell_u = 0$ holds for all $u \in V_+^{\mathrm{l}}(o,u_1)\setminus\{o,u_1\}$ and we choose u_3 such that $\ell_u = 0$ holds for all $u \in V_+^{\mathrm{l}}(u_3,w)\setminus\{u_3\}$. We now consider a flow decomposition as in Lemma 2. Due to $q \geq 0$, an exit $v_3 \in V_-^{\mathrm{l}}(u_3,w)$ with $q(P^{\mathrm{l}}(u_3,v_3)) > 0$ exists. Moreover, by the choice of u_1, there is an exit $v_1 \in V_-^{\mathrm{l}}(u_1,w)$ with $\ell_v = 0$ for all $v \in V_-^{\mathrm{l}}(o,v_1)\setminus\{v_1\}$ and $q(P^{\mathrm{l}}(u_1,v_1)) > 0$. We need to distinguish two cases.

Case 1: $v_1 \prec_\mathrm{l} u_2$ holds. We now decrease $q(P^{\mathrm{l}}(u_3,v_3))$ by $\varepsilon > 0$ and increase $q(P^{\mathrm{l}}(u_2,v_3))$ by the same amount ε. This increases the potential difference $\Pi_{P^{\mathrm{l}}(o,w)}(q)$ due to $u_2 \prec_\mathrm{l} u_3$. Thus, we decrease $q(P^{\mathrm{l}}(u_1,v_1))$ by $\tilde{\varepsilon} > 0$. Due to Lemma 4, we can choose ε and $\tilde{\varepsilon}$ such that $\Pi_{P^{\mathrm{l}}(o,w)}(q)$ stays the same as before the modification and $\ell_{u_1} > 0, \ell_{u_2} \leq b_{u_2}, \ell_{u_3} > 0, \ell_{v_1} > 0$ holds. In particular, the binary variables of z stay the same. Due to this and Lemmas 22–24, the values of f_2, f_3, and f_4 stay the same. Moreover, the modified solution satisfies Constraints (17b). Furthermore, by this modification we decrease q_a for $a \in P^{\mathrm{l}}(u_1,v_1)$, increase q_a for $a \in P^{\mathrm{l}}(u_2,u_3)$, and the remaining arc flows stay the same. Hence, since $u_1 \prec_\mathrm{l} v_1 \prec_\mathrm{l} u_2 \prec_\mathrm{l} u_3$ and by Lemma 4(d), we possibly increase the potential difference between w_1 and w_2 and Constraint (17d) is still satisfied. Consequently, z is still feasible for (17). Due to this modification, we decrease $\ell_{u_1} > 0$ and $\ell_{u_3} > 0$ and increase ℓ_{u_2}. By Lemma 21, considering only the decrease of ℓ_{u_1} and ℓ_{u_3} does not change the objective function value. In contrast, the increase of ℓ_{u_2} decreases f_1 because

$$x_{u_1}^{\preccurlyeq_\mathrm{l}} x_{u_3}^{\succcurlyeq_\mathrm{l}} \sum_{v \in V_+^{\mathrm{l}}(u_1,u_3)\setminus\{u_1,u_3\}} (b_v - \ell_v)$$

decreases. Thus, the modification decreases the objective function value, which contradicts the optimality of the original solution.

Case 2: $u_2 \prec_l v_1$ holds. We now decrease $q(P^l(u_1, v_1))$ by $\varepsilon > 0$ and increase $q(P^l(u_2, v_1))$ by the same amount ε. This decreases the potential difference $\Pi_{P^l(o,w)}(q)$ due to $u_1 \prec_l u_2$. Thus, we now decrease $q(P^l(u_3, v_3))$ by $\tilde{\varepsilon} > 0$ and increase $q(P^l(u_2, v_3))$ by the same amount $\tilde{\varepsilon}$, which increases the potential difference $\Pi_{P^l(o,w)}(q)$ due to $u_2 \prec_l u_3$. Due to Lemma 4, we can choose ε and $\tilde{\varepsilon}$ such that $\Pi_{P^l(o,w)}(q)$ stays the same and $\ell_{u_1} > 0, \ell_{u_2} \le b_{u_2}, \ell_{u_3} > 0$ holds. In analogy to Case 1, the function values of f_2, f_3, and f_4 stay the same and the modified solution satisfies Constraints (17b). Furthermore, the modification only decreases q_a for $a \in P^l(u_1, u_2)$ and increases flow q_a for $a \in P^l(u_2, u_3)$. The remaining arc flows stay the same. Hence, since $u_1 \prec_l u_2 \prec_l u_3$ and by Lemma 4(d), we possibly increase the potential difference between w_1 and w_2 and Constraint (17d) is still satisfied. Consequently, z is feasible for (17) after modification. In analogy to Case 1, the modification decreases f_1, which contradicts the optimality of the original solution. ∎

Lemma 26. *If z is an optimal solution of (17), then $f_2(\ell, y^{\preccurlyeq_l}) = 0$ holds.*

Proof. Let z be an optimal solution of (17). By contradiction, we assume that $f_2(\ell, y^{\preccurlyeq_l}) > 0$ holds. Lemma 18 implies that ℓ does not satisfy Property (b). Consequently, there are exits $v_1, v_2 \in V_-^l(o, w)$ with $v_1 \prec_l v_2$, $\ell_{v_1} > 0$ and $\ell_{v_2} < b_{v_2}$. We now choose v_1 such that $\ell_u = 0$ holds for all $u \in V_-^l(o, v_1) \setminus \{v_1\}$ and v_2 such that $\ell_u = b_u$ holds for all $u \in V_-^l(v_1, v_2) \setminus \{v_1, v_2\}$. Next, let an entry $u_1 \in V_+^l(o, w)$ be given so that $\ell_{u_1} > 0$, $\ell_u = 0$ for all $u \in V_+^l(o, u_1) \setminus \{o, u_1\}$, and in a flow decomposition as by Lemma 2, $q(P^l(u_1, v_1)) > 0$ holds. Due to Lemma 4 and $v_1 \prec_l v_2$, we can decrease $q(P^l(u_1, v_1))$ and increase $q(P^l(u_1, v_2))$ such that $\Pi_{P^l(o,w)}(q)$ remains the same and $0 < \ell_{u_1} \le b_{u_1}, \ell_{v_1} > 0, 0 < \ell_{v_2} \le b_{v_2}$ hold. Thus, the binary variables of z stay the same. Furthermore, by Lemmas 21, 23, and 24 the values of f_1, f_3, and f_4 stay the same. The modified solution satisfies Constraints (17b) and we only decrease q_a for $a \in P^l(u_1, v_1)$ and increase q_a for $a \in P^l(v_1, v_2)$. The remaining arc flows are unchanged. Then, since $u_1 \prec_l v_1 \prec_l v_2$ and by Lemma 4(d), Constraint (17d) is still satisfied. Consequently, z is still feasible for (17). Due to this modification, we decrease $\ell_{v_1} > 0$ and increase ℓ_{v_2}. By Lemma 22, considering only the decrease of ℓ_{v_1} does not change the objective function value. In contrast, the increase of ℓ_{v_2} decreases f_2 because

$$y_{v_1}^{\preccurlyeq_l} \sum_{v \in V_-^l(v_1, w) \setminus \{v_1\}} (b_v - \ell_v)$$

decreases. Thus, the modification decreases the objective function value, which contradicts the optimality of the original solution. ∎

Lemma 27. *If z is an optimal solution of (17), then $f_3(\ell, x^{\succcurlyeq_r}) = 0$ holds.*

Lemma 28. *If z is an optimal solution of (17), then $f_4(\ell, y^{\preccurlyeq_r}, y^{\succcurlyeq_r}) = 0$ holds.*

Again, the proofs for the results concerning f_3 and f_4 can be found in Appendix A. Finally, we obtain the main structural property for nodes w_1 and w_2 on different sides of G by combining the previous lemmas.

Theorem 29. *Let $(o, w) \in V_+ \times V_-$ be fixed, $w_1 \in P^l(o, w)$, and $w_2 \in P^r(o, w)$. Then, an optimal solution (ℓ, q, π) of (14) exists that satisfies Properties (a)–(d).*

Proof. The zero nomination is feasible for Problem (14). Furthermore, the feasible region of the latter problem is compact and thus an optimal solution is attained. Consequently, Problem (17) has an optimal solution, which is attained. Due to Lemmas 25–28 and 17–20, an optimal solution (ℓ, q, π, x, y) of Problem (17) exists that satisfies Properties (a)–(d). Additionally, the solution (ℓ, q, π) is also optimal for Problem (14). ∎

5.2 | Nodes on the same side of G

Assume $w_1, w_2 \in P^l(o, w)$ or $w_1, w_2 \in P^r(o, w)$ holds. We can w.l.o.g. assume that $w_1, w_2 \in P^r(o, w)$ holds. If $w_2 \prec_r w_1$ holds, then from $q \ge 0$ in Problem (14) it follows that $\Pi_{P^r(w_1, w_2)}(q) \le 0$ is valid. Thus, the zero nomination is an optimal solution for Problem (14). Consequently, we now assume that $w_1 \prec_r w_2$ holds.

We want to show that an optimal solution (ℓ, q, π) of Problem (14) exists such that Properties (a), (b), (d), and (a) w.r.t. $P^r(o, w)$ are satisfied, i.e., two entries $s_1^r, s_2^r \in V_+^r(o, w)$ with $s_1^r \preccurlyeq_r s_2^r$ exists such that

$$\begin{aligned} \ell_v &= 0, \quad v \in (V_+^r(o, s_1^r) \cup V_+^r(s_2^r, w)) \setminus \{o, s_1^r, s_2^r\}, \\ \ell_v &= b_v, \quad v \in V_+^r(s_1^r, s_2^r) \setminus \{s_1^r, s_2^r\}, \end{aligned}$$

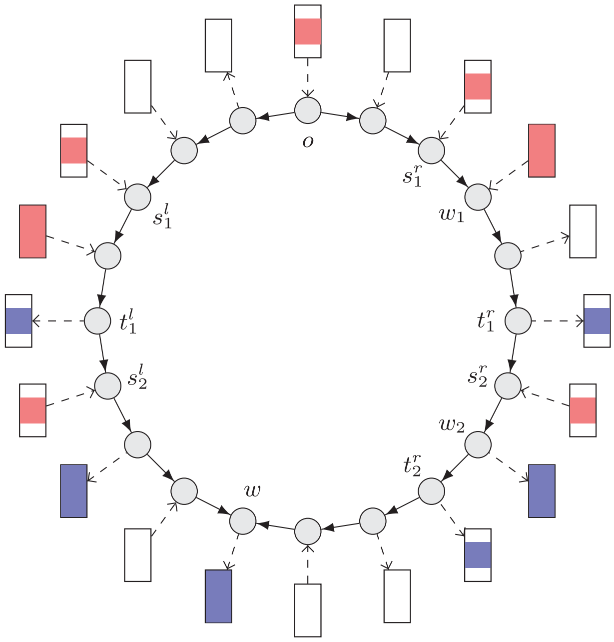

FIGURE 4 Configuration of s and t nodes with $o \preccurlyeq_{\mathrm{r}} w_1 \prec_{\mathrm{r}} w_2 \preccurlyeq_{\mathrm{r}} w$. Boxes qualitatively illustrate the amount of the booking that is nominated

is satisfied. Figure 4 illustrates a possible node configuration. To this end, we introduce an optimization problem similar to (16), which is given by

$$\min_{\ell,q,\pi,x,y} \quad f_1(\ell, x^{\preccurlyeq_{\mathrm{l}}}, x^{\succcurlyeq_{\mathrm{l}}}) + f_2(\ell, y^{\preccurlyeq_{\mathrm{l}}}) + f_3(\ell, x^{\preccurlyeq_{\mathrm{r}}}, x^{\succcurlyeq_{\mathrm{r}}}) + f_4(\ell, y^{\preccurlyeq_{\mathrm{r}}}, y^{\succcurlyeq_{\mathrm{r}}}) \tag{22a}$$

$$\text{s.t.} \quad \text{(1a), (3b), (14b), (14c), (16b)–(16h), (17d),}$$

$$M x_v^{\preccurlyeq_{\mathrm{r}}} \geq \sum_{u \in V_+^{\mathrm{r}}(o,v)\setminus\{o\}} \ell_u, \quad v \in V_+^{\mathrm{r}}(o,v)\setminus\{o\}, \tag{22b}$$

$$x_v^{\preccurlyeq_{\mathrm{r}}} \in \{0,1\}, \quad v \in V. \tag{22c}$$

Note that an analogous variant of Lemma 16 is also valid for Problem (22).

We specify the parts of the objective function of (22) as follows: the functions f_1, f_2, and f_4 are defined as in Lemmas 17, 18, and 20. The function f_3 is defined in analogy to Lemma 17 w.r.t. P^{r}. We note that f_i for $i = 1, \ldots, 4$ also inherit the corresponding properties of Lemmas 17–24. We now prove that the optimal objective value of (22) is zero.

Lemma 30. *If z is an optimal solution of (22), then $f_1(\ell, x^{\preccurlyeq_{\mathrm{l}}}, x^{\succcurlyeq_{\mathrm{l}}}) = 0$ holds.*

Proof. The claim follows in analogy to Lemma 25. In doing so, we note that the modifications in the proof of Lemma 25 only affect nodes of $P^{\mathrm{l}}(o, w)$. Consequently, we do not change the potential difference between w_1 and w_2 due to $w_1, w_2 \in P^{\mathrm{r}}(o, w)$. ∎

Lemma 31. *If z is an optimal solution of (22), then $f_2(\ell, y^{\preccurlyeq_{\mathrm{l}}}) = 0$ holds.*

Proof. The claim follows in analogy to Lemma 26. ∎

To show analogous results for f_3 and f_4, we make use of an auxiliary lemma.

Lemma 32. *An optimal solution z of (22) exists such that $\ell_v = 0$ for all $v \in V_-^{\mathrm{r}}(o, w_1)$ and $\ell_u = 0$ for all $u \in V_+^{\mathrm{r}}(w_2, w)$ is satisfied.*

Proof. We choose an optimal solution z of (22) such that

$$\sum_{v \in V_-^{\mathrm{r}}(o,w_1)} \ell_v + \sum_{u \in V_+^{\mathrm{r}}(w_2,w)} \ell_u$$

is minimal. Note that every addend is nonnegative. By contradiction, we assume that

$$\sum_{v\in V_-^{\mathrm{r}}(o,w_1)} \ell_v + \sum_{u\in V_+^{\mathrm{r}}(w_2,w)} \ell_u > 0$$

holds.

Case 1: There exists $v \in V_-^{\mathrm{r}}(o,w_1)$ with $\ell_v > 0$. We now choose v such that $\ell_{v'} = 0$ for all $v' \in V_-^{\mathrm{r}}(o,v)\backslash\{v\}$ is satisfied. Consequently, an entry $u \in V_+^{\mathrm{r}}(o,v)$ exists such that $\ell_{u'} = 0$ holds for all $u' \in V_+^{\mathrm{r}}(o,u)\backslash\{o\}$ and in a flow decomposition, such as in Lemma 2, $q(P^{\mathrm{r}}(u,v)) > 0$ is satisfied. We can now decrease the latter by $\varepsilon > 0$ such that $\ell_u > 0$ and $\ell_v > 0$ holds. This decreases the potential drop $\Pi_{P^{\mathrm{r}}(o,w)}(q)$. Due to Lemmas 30 and 31, we can assume that $q(P^{\mathrm{l}}(s_1^l,t_1^l)) > 0$ holds. By using Lemma 4, we can now decrease the latter by $\tilde{\varepsilon}$ and choose ε such that $\Pi_{P^{\mathrm{l}}(o,w)}(q) = \Pi_{P^{\mathrm{r}}(o,w)}(q)$ holds and $\ell_u, \ell_v, \ell_{s_1^l}, \ell_{t_1^l}$ are positive. Moreover, Lemmas 21–24 imply that the solution obtained after the modifications is still feasible and optimal for (22). In doing so, we note that the modifications do not change any flow of $P^{\mathrm{r}}(w_1,w_2)$ and thus the potential difference between w_1 and w_2 stays the same. This is a contradiction to the choice of z because

$$\sum_{v\in V_-^{\mathrm{r}}(o,w_1)} \ell_v + \sum_{u\in V_+^{\mathrm{r}}(w_2,w)} \ell_u$$

is decreased in the modified solution.

Case 2: There is $u \in V_+^{\mathrm{r}}(w_2,w)$ with $\ell_u > 0$. We now choose u such that $\ell_{u'} = 0$ for all $u' \in V_+^{\mathrm{r}}(u,w)$. Due to $q \geq 0$, an exit $v \in V_-^{\mathrm{r}}(u,w)$ exists such that $\ell_{v'} = 0$ holds for all $v' \in V_-^{\mathrm{r}}(v,w)\backslash\{v,w\}$ and $q(P^{\mathrm{r}}(u,v)) > 0$. In analogy to Case 1, the claim follows by decreasing the flow $q(P^{\mathrm{r}}(u,v))$ by $\varepsilon > 0$ and $q(P^{\mathrm{l}}(s_1^l,t_1^l))$ by $\tilde{\varepsilon} > 0$. ■

Lemma 33. *If z is an optimal solution of (22), then $f_3(\ell, x^{\leqslant_{\mathrm{r}}}, x^{\geqslant_{\mathrm{r}}}) = 0$ holds.*

Proof. Let z be an optimal solution of (22) that satisfies Lemma 32. By contradiction, we assume that $f_3(\ell, x^{\leqslant_{\mathrm{r}}}, x^{\geqslant_{\mathrm{r}}}) > 0$ holds. Lemma 17 implies that ℓ does not satisfy Property (a) w.r.t. P^{r}. Consequently, there are entries $u_1,u_2,u_3 \in V_+^{\mathrm{r}}(o,w)\backslash\{o\}$ with $u_1 \prec_{\mathrm{r}} u_2 \prec_{\mathrm{r}} u_3$ such that $\ell_{u_1} > 0, \ell_{u_2} < b_{u_2}$, and $\ell_{u_3} > 0$ hold. If $q_a > 0$ for $a \in \delta^{\mathrm{out}}(o) \cap P^{\mathrm{r}}(o,w)$, we replace $u_1 = o$. Otherwise, we choose $u_1 \neq o$ such that $\ell_u = 0$ holds for all $u \in V_+^{\mathrm{r}}(o,u_1)\backslash\{o,u_1\}$ and we choose u_3 such that $\ell_u = 0$ holds for all $u \in V_+^{\mathrm{r}}(u_3,w)\backslash\{u_3\}$. We now consider a flow decomposition as in Lemma 2. Due to $q \geq 0$, an exit $v_3 \in V_-^{\mathrm{r}}(u_3,w)$ with $q(P^{\mathrm{r}}(u_3,v_3)) > 0$ exists. By the choice of u_1, there is an exit $v_1 \in V_-^{\mathrm{r}}(u_1,w)$ with $\ell_v = 0$ for all $v \in V_-^{\mathrm{r}}(o,v_1)\backslash\{v_1\}$ and $q(P^{\mathrm{r}}(u_1,v_1)) > 0$. Consequently, $v_1 \leqslant_{\mathrm{r}} v_3$ holds. We now distinguish two cases.

Case 1: $u_2 \leqslant_{\mathrm{r}} w_1$. Due to Lemma 32, $w_1 \leqslant_{\mathrm{r}} v_1$ holds. Consequently, we can decrease $q(P^{\mathrm{r}}(u_1,v_1)) > 0$ by $\varepsilon > 0$ and we increase $q(P^{\mathrm{r}}(u_2,v_1))$ by the same amount such that $\ell_{u_1} > 0$ and $\ell_{u_2} \leq b_{u_2}$ holds. Since $u_1 \prec_{\mathrm{r}} u_2$ holds, this modification decreases the potential difference $\Pi_{P^{\mathrm{r}}(o,w)}(q)$ but the flow on arcs of $P^{\mathrm{r}}(w_1,w_2)$ stays the same due to $u_2 \leqslant_{\mathrm{r}} w_1$. Consequently, $\Pi_{P^{\mathrm{r}}(w_1,w_2)}(q)$ is unchanged. From the proof of Lemma 25, it follows that this modification decreases f_3. In analogy to Case 1 of Lemma 32, we can now decrease $\Pi_{P^{\mathrm{l}}(o,w)}(q)$ by modifying $\ell_{s_1^l}$ and $\ell_{t_1^l}$ such that $\Pi_{P^{\mathrm{r}}(o,w)}(q) = \Pi_{P^{\mathrm{l}}(o,w)}(q)$ holds without changing the values of f_i for $i = 1, \ldots, 4$. This is a contradiction to the optimality of z because we have decreased f_3 in the first part of the modification.

Case 2: $w_1 \prec_{\mathrm{r}} u_2$. Due to $u_2 \prec_{\mathrm{r}} u_3$ and Lemma 4, we can decrease $q(P^{\mathrm{r}}(u_3,v_3))$ by $\varepsilon > 0$ and increase $q(P^{\mathrm{r}}(u_2,v_3))$ by $0 < \tilde{\varepsilon} \leq \varepsilon$ such that $\Pi_{P^{\mathrm{r}}(o,w)}(q) = \Pi_{P^{\mathrm{l}}(o,w)}(q)$, $\ell_{u_3} > 0$, $\ell_{v_3} > 0$, and $\ell_{u_2} \leq b_{u_2}$ holds. Consequently, the binary variables of z stay the same. By using Lemmas 21, 22, and 24, the values f_1, f_2, and f_4 stay the same as well. The modified solution satisfies Constraints (17b). Furthermore, the modification only increases q_a for $a \in P^{\mathrm{r}}(u_2,u_3)$ and decreases the flow q_a for $a \in P^{\mathrm{r}}(u_3,v_3)$. The remaining arc flows stay unchanged. Due to $w_1 \prec_{\mathrm{r}} u_2 \prec_{\mathrm{r}} u_3 \prec_{\mathrm{r}} w_2$ and Lemma 4(d), we possibly increase the potential difference between w_1 and w_2 and thus Constraint (17d) is still satisfied. Case 1 of Lemma 25 implies that the previous modification decreases f_3, which is a contradiction to the optimality of z. ■

Lemma 34. *If z is an optimal solution of (22), then $f_4(\ell, y^{\leqslant_{\mathrm{r}}}, y^{\geqslant_{\mathrm{r}}}) = 0$ holds.*

Proof. Let z be an optimal solution of (22) that satisfies Lemma 32. By contradiction, we assume that $f_4(\ell, y^{\leqslant_{\mathrm{r}}}, x^{\geqslant_{\mathrm{r}}}) > 0$ holds. Lemma 20 implies that ℓ does not satisfy Property (d). Consequently, there are exits $v_1,v_2,v_3 \in V_-^{\mathrm{r}}(o,w)\backslash\{w\}$ with $v_1 \prec_{\mathrm{r}} v_2 \prec_{\mathrm{r}} v_3$, $\ell_{v_1} > 0, \ell_{v_2} < b_{v_2}$, and $\ell_{v_3} > 0$. Furthermore, we choose v_1 such that $\ell_v = 0$ holds for all $v \in V_-^{\mathrm{r}}(o,v_1)\backslash\{v_1\}$. If $q_a > 0$ for $a \in \delta^{\mathrm{in}}(w) \cap P^{\mathrm{r}}(o,w)$, we replace $v_3 = w$. Otherwise, we choose $v_3 \neq w$ such that $\ell_v = 0$ holds for all $v \in V_-^{\mathrm{l}}(v_3,w)\backslash\{v_3,w\}$. We now consider a flow decomposition as in Lemma 2. Due to $q \geq 0$, there is an entry $u_3 \in V_+^{\mathrm{r}}(o,v_3)$ with $\ell_u = 0$ for all $u \in V_+^{\mathrm{r}}(u_3,w)\backslash\{u_3\}$ and $q(P^{\mathrm{r}}(u_3,v_3)) > 0$. Furthermore, an entry $u_1 \in V_+^{\mathrm{r}}(o,w)$ with $\ell_u = 0$ for all $u \in V_+^{\mathrm{r}}(o,u_1)\backslash\{o,u_1\}$ exists that satisfies $q(P^{\mathrm{r}}(u_1,v_1)) > 0$. Due to Lemma 32, $w_1 \prec_{\mathrm{r}} v_1 \prec_{\mathrm{r}} v_2 \prec_{\mathrm{r}} v_3$ holds. We now distinguish two cases.

Case 1: $v_2 \preccurlyeq_r w_2$. Consequently, $v_1 \prec_r v_2 \preccurlyeq_r w_2$ holds. We can now decrease $q(P^r(u_1, v_1))$ by $\varepsilon > 0$ and increase $q(P^r(u_1, v_2))$ by $0 < \tilde{\varepsilon} \leq \varepsilon$ such that $\Pi_{P^r(o,w)}$ stays the same and $\ell_{u_1} > 0, \ell_{v_1} > 0$, and $\ell_{v_2} \leq b_{v_2}$ holds. In particular, the binary variables of z stay the same after the modification. Due to this and Lemmas 21 and 23, the values of f_1, f_2, and f_3 stay unchanged. The modified solution satisfies Constraints (17b). Furthermore, this modification only decreases q_a for $a \in P^r(u_1, v_1)$ and increases arc flows q_a for $a \in P^r(v_1, v_2)$. The remaining arc flows stay the same. Hence, since $w_1 \prec_r v_1 \prec_r v_2 \preccurlyeq_r w_2$ and by Lemma 4(d), we possibly increase the potential difference between w_1 and w_2 and Constraint (17d) is still satisfied. Consequently, z is still feasible for (22). In analogy to Case 1 of Lemma 28, it follows that the modification decreases f_4, which is a contradiction to the optimality of z.

Case 2: $w_2 \prec_r v_2$. Consequently, $u_3 \prec_r w_2 \prec_r v_2 \prec_r v_3$ holds. We can now apply Case 2 of Lemma 28. In doing so, we keep in mind that $w_1 \prec_r v_1$ and $w_2 \prec_r v_2 \prec_r v_3$ hold which ensures that z still satisfies (17d) after the applied modifications. ■

Finally, we obtain a result for the present case that is analogous to Theorem 29.

Theorem 35. *Let $(o, w) \in V_+ \times V_-$ be fixed and $w_1, w_2 \in P^r(o, w)$. Then, an optimal solution (ℓ, q, π) of (14) exists that satisfies Properties (a), (b), (d), and (a) w.r.t. P^r.*

Proof. The zero nomination is feasible for Problem (14) and it is optimal if $w_2 \preccurlyeq_r w_1$ holds. Furthermore, the feasible region of the latter problem is compact and thus an optimal solution is attained. Consequently, Problem (22) has an optimal solution, which is attained. Due to Lemmas 30–34 and Lemmas 17–20, for $w_1 \prec_r w_2$ an optimal solution of Problem (22) exists that satisfies Properties (a), (b), (d) and, (a) w.r.t. P^r. Additionally, the solution is also optimal for Problem (14). ■

6 | A POLYNOMIAL-TIME ALGORITHM

Exploiting the special structure of nominations that maximize the potential difference between a pair of nodes, we now show that the feasibility of a booking can be checked in polynomial time on a cycle. First, we obtain an estimate on the number of arithmetic operations necessary to detect the existence of an infeasible nomination, or otherwise certify its nonexistence. In a second step, we then translate this result to the Turing model of computation, resulting in a polynomial-time algorithm for deciding the feasibility of a booking. For doing so, we make the following nonrestrictive assumption on the rationality of the problem data.

Assumption 36. *We consider a booking $b \in \mathbb{Q}^V$ and assume that $\Lambda_a \in \mathbb{Q}$ for all $a \in A$ and $\pi_u^-, \pi_u^+ \in \mathbb{Q}$ for all $u \in V$. Additionally, we assume that the encoding lengths are bounded from above by τ.*

As a consequence of Corollary 15, a booking b is feasible if and only if, for every $(w_1, w_2) \in V^2$ and $(o, w) \in V_+ \times V_-$,

$$\pi_{w_1} - \pi_{w_2} > \pi_{w_1}^+ - \pi_{w_2}^-, \quad \text{(1a), (3b), (14b), (14c)} \tag{23}$$

admits no solution. We now make several observations. First, recall that A' is obtained from A by orienting all arcs from o to w. Then, given (14c), the right-hand sides of (14b) simplify to $\Lambda_a q_a^2$ for all $a \in A'$. Second, we eliminate the potentials π by aggregating the resulting constraints along $P^l(o, w)$ and $P^r(o, w)$. We only treat the situation corresponding to Section 5 in which $o \preccurlyeq_r w_1 \prec_r w_2 \preccurlyeq_r w$ is valid, since it has the highest number of s and t nodes necessary to set up the structural properties and thus represents the worst case in terms of complexity. The situation corresponding to Section 5 with w_1 and w_2 on different paths w.r.t. o and w can however be treated in a similar way. We obtain

$$\sum_{a \in P^r(w_1, w_2)} \Lambda_a q_a^2 > \pi_{w_1}^+ - \pi_{w_2}^-,$$
$$\sum_{a \in P^l(o,w)} \Lambda_a q_a^2 - \sum_{a \in P^r(o,w)} \Lambda_a q_a^2 = 0.$$

It is well known that if the nomination is balanced, the rank of the flow conservation constraints (1a) is $|V| - 1$, resulting in a single degree of freedom in the case of a cycle. Thus, we introduce $\ell_w = \ell_w^l + \ell_w^r$ to take into account the supply to the flow-meeting point w along P^l and P^r separately. Then, for $a = (u, v) \in A'$, (1a) leads to

$$q_a = \begin{cases} -\sum_{v' \in P^l(v,w) \setminus \{w\}} \sigma_{v'} \ell_{v'} + \ell_w^l, & \text{if } a \in P^l(o, w), \\ -\sum_{v' \in P^r(v,w) \setminus \{w\}} \sigma_{v'} \ell_{v'} + \ell_w^r, & \text{if } a \in P^r(o, w). \end{cases}$$

As a consequence of the previous discussion, we need to check that the system of polynomials

$$\sum_{a=(u,v)\in P^{\mathrm{r}}(w_1,w_2)} \Lambda_a \left(- \sum_{v'\in P^{\mathrm{r}}(v,w)\setminus\{w\}} \sigma_{v'}\ell_{v'} + \ell^{\mathrm{r}}_w \right)^2 > \pi^+_{w_1} - \pi^-_{w_2}, \tag{24a}$$

$$\sum_{a=(u,v)\in P^{\mathrm{l}}(o,w)} \Lambda_a \left(- \sum_{v'\in P^{\mathrm{l}}(v,w)\setminus\{w\}} \sigma_{v'}\ell_{v'} + \ell^{\mathrm{l}}_w \right)^2 - \sum_{a=(u,v)\in P^{\mathrm{r}}(o,w)} \Lambda_a \left(- \sum_{v'\in P^{\mathrm{r}}(v,w)\setminus\{w\}} \sigma_{v'}\ell_{v'} + \ell^{\mathrm{r}}_w \right)^2 = 0, \tag{24b}$$

$$- \sum_{v'\in P^{\mathrm{l}}(v,w)\setminus\{w\}} \sigma_{v'}\ell_{v'} + \ell^{\mathrm{l}}_w \geq 0, \quad (u,v)\in P^{\mathrm{l}}, \tag{24c}$$

$$- \sum_{v'\in P^{\mathrm{r}}(v,w)\setminus\{w\}} \sigma_{v'}\ell_{v'} + \ell^{\mathrm{r}}_w \geq 0, \quad (u,v)\in P^{\mathrm{r}}, \tag{24d}$$

$$\ell^{\mathrm{l}}_w + \ell^{\mathrm{r}}_w = \ell_w, \qquad \ell \in N(b), \tag{24e}$$

admits no solution.

We now reduce the dimension of (24) to obtain a system of polynomials with a constant number of constraints and variables independent of the problem size. Hence, we make use of the structure analyzed in Section 5 for potential-difference maximizing nominations.

In what follows, we consider a configuration of Properties (a), (b), (d) and (a) w.r.t. P^{r}, determined by $s^l_1, s^l_2 \in V^{\mathrm{l}}_+(o,w)$, $t^l_1 \in V^{\mathrm{l}}_-(o,w)$, $s^r_1, s^r_2 \in V^{\mathrm{r}}_+(o,w)$ as well as $t^r_1, t^r_2 \in V^{\mathrm{r}}_-(o,w)$, and the corresponding partially fixed $\ell \in N(b)$.

Lemma 37. *There exists a system of polynomials equivalent to (24e) that has at most nine variables and 16 constraints, independent of the size of the cycle.*

Proof. First, observe that we can substitute the nomination entries for o and w using

$$\ell_w = \ell^{\mathrm{l}}_w + \ell^{\mathrm{r}}_w, \quad \ell_o = - \sum_{u\in V\setminus\{o\}} \sigma_u \ell_u.$$

Fixing nomination entries either to their booking bound or to zero, as by Properties (a)–(d), it is easy to observe that $\ell_{s^l_1}, \ell_{s^l_2}, \ell_{t^l_1}, \ell_{s^r_1}, \ell_{s^r_2}, \ell_{t^r_1}, \ell_{t^r_2}, \ell^{\mathrm{l}}_w, \ell^{\mathrm{r}}_w$, are the only remaining 9 variables. Note that in some situations these variables may coincide. In particular, there are at most 14 constraints corresponding to the booking bounds, namely $0 \leq \ell_u \leq b_u$ for all $u \in \{s^l_1, s^l_2, t^l_1, s^r_1, s^r_2, t^r_1, t^r_2\}$.

The number of additional constraints due to o and w depend on the configuration under consideration. If $o \notin \{s^l_1, s^r_1\}$, then the additional constraint $\ell_o = b_o$ is necessary. If $w \notin \{t^l_1, t^r_2\}$, then $\ell_w = b_w$ is required. ■

A combinatorial analysis of (24c) and (24d) also leads to the following constant number of constraints.

Lemma 38. *There exists a system of polynomials equivalent to (24c) and (24d) with at most 24 constraints, independent of the size of the cycle. This system can be determined in $O(|A|)$ time.*

Proof. Let us first consider (24d). There are four s and t nodes on $P^{\mathrm{r}}(o,w)$, namely $s^r_1, s^r_2, t^r_1, t^r_2$. Thus, assuming that constants have been moved to the right-hand sides in (24d), there can be at most 2^4 left-hand sides with different constant right-hand sides. For every left-hand side, it is sufficient to impose a single constraint admitting the maximum constant on the right-hand side. This is easily achieved by iterating over all arcs of $P^{\mathrm{r}}(o,w)$. Similarly, (24c) can be reduced to a system with 2^3 constraints. ■

The following result now is a direct consequence of the two previous results.

Theorem 39. *System (24) can be reduced in $O(|A|)$ time to a system of polynomials with at most nine variables and 42 constraints.*

Next, we apply a general decision algorithm for the existence of solutions for systems of polynomial equations and inequalities, given by Algorithm 14.16 in [5], to estimate the number of arithmetic operations necessary to decide the existence of a solution for (24). Note that this algorithm can in particular handle strict inequalities as required to determine a violation of the potential difference bounds; see, e.g., Notation 11.31 in [5]. We then obtain the following result.

Theorem 40. *Suppose Assumption 36 holds. Then, the existence of a solution of (24) can be decided in* $O((\log |V| + \tau)|V_+|^4|V_-|^3)$ *time.*

Proof. Algorithm 14.16 in [5] has a complexity in the arithmetic computation model of $s^k d^{O(k)}$, where s is the number of constraints, k is the number of variables, and d is the highest degree of the polynomials. For a given configuration of Properties (a), (b), (d), and (a) w.r.t. P^{r}, the number of variables and constraints in (24) can be reduced to a constant by Theorem 39 and $d = 2$. Consequently, the existence of a solution for this reduced system can be checked in $O(1)$ arithmetic operations.

Under Assumption 36, the encoding lengths of the rational coefficients of (24) are bounded by $O(\log |V| + \tau)$. This can easily be deduced by analyzing the constant term in, e.g., (24a). Given the constant number of variables and constraints in the reduced version of (24), the encoding length of integer coefficients after scaling is still bounded by $O(\log |V| + \tau)$. In this case, the encoding length of coefficients appearing in intermediate computations and the output of Algorithm 14.16 in [5] are also bounded by $O(\log |V| + \tau)$. From a discussion in Chapter 1 of [20], the existence of a solution to the reduced version of System (24) can then be checked in $O(\log |V| + \tau)O(1) = O(\log |V| + \tau)$ time on a Turing machine.

By Lemmas 30–34, a solution of (24) exists if and only if there is a configuration of Properties (a), (b), (d), and (a) w.r.t. P^{r}, such that a solution of the reduced version of (24) exists. Consequently, the result follows by iterating over all combinations of $s_1^l, s_2^l, t_1^l, s_1^r, s_2^r, t_1^r, t_2^r$. ∎

Furthermore, iterating this procedure over all $(o, w) \in V_+ \times V_-$, we obtain the final result for validating a booking on a cycle, which ensures that checking the feasibility of a booking on a cycle can be done in polynomial time.

Corollary 41. *Under Assumption 36, the feasibility of booking* $b \in \mathbb{Q}_{\geq 0}^V$ *can be checked in* $O((\log |V| + \tau)|V_+|^5|V_-|^4)$ *time on a cycle.*

We close this section with a short remark on how our results can be applied to other types of utility networks, e.g., to water distribution or power networks.

Remark. The structural properties derived in Sections 2–5 can be applied to potential-based networks if the following assumptions hold: The potentials satisfy (1) where for any arc $a \in A$, the right-hand side of (1b) is a function $\phi_a : \mathbb{R} \to \mathbb{R}$ that may depend on the arc flow q_a and that is continuous, strictly increasing, and odd, i.e., $\phi_a(-q_a) = -\phi_a(q_a)$. Consequently, our structural results hold for many different networks such as water, hydrogen, or lossless DC (direct current) power flow networks, if the physics model is chosen appropriately; see [19]. In particular, we can reduce the optimization problem (3), where we replace the right-hand side of (1b) by ϕ_a, to a fixed inequality system for all these potential-based networks as shown in Section 5. However, the presented complexity result is only valid in the case in which the potential function $\phi_a(q_a)$ is a polynomial in the variables $|q_a|$ and q_a that is strictly increasing and odd.

However, the overall question of deciding the feasibility of a booking discussed in this article is rather specific and tailored to the European gas market system since, e.g., the market design for electricity is different from the one for gas in Europe.

7 | CONCLUSION

In this work, we prove that deciding the feasibility of a booking in the European entry-exit gas market model is in P for the special case of cycle networks. To the best of our knowledge, this is the first in-depth complexity analysis in this context that considers a nonlinear flow model and a network topology that is not a tree. Our approach requires the combination of both the cyclic structure of the network and properties of the underlying nonlinear potential-based flow model with a general decision algorithm from real algebraic geometry. We show that the size of a polynomial equality and inequality system for deciding the feasibility of a booking is constant and, in particular, does not depend on the size of the cycle. Thus, a general algorithm for solving this system can serve as a constant-time oracle used in an enumeration of polynomial complexity.

Although our theoretical result moves the frontier of knowledge about the hardness of deciding the feasibility of bookings in the European entry-exit gas market, it still remains an open question to exactly determine the frontier between easy and hard cases if a nonlinear and potential-based flow model is considered. Although we believe that the problem is hard on general networks, no hardness results are known so far. Since both trees and single cycle networks are now well understood, a possibility is to consider more general classes of networks. Thus, a reasonable next step could be networks consisting of a single cycle with trees on it or, even more generally, cactus graphs. In our opinion, it is promising to combine the techniques used on trees and cycles in order to solve this larger graph class.

Finally, although the present article is a very specific one, we hope that the structural insights gained can be later put together with other insights to obtain more general techniques for (adjustable) robust and nonlinear flow problems.

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APPENDIX A : OMITTED PROOFS

Proof of Lemma 19. Let z be feasible for (17). For $i \in V_+^{\mathrm{r}}(o, w)$,

$$x_i^{\succcurlyeq_{\mathrm{r}}} \sum_{v \in V_+^{\mathrm{r}}(o,i) \setminus \{i\}} (b_v - \ell_v) \geq 0$$

holds. Assume now that Property (c) does not hold. Consequently, there are $u_1, u_2 \in V_+^{\mathrm{r}}(o, w)$ with $u_1 \prec_{\mathrm{r}} u_2$ such that $\ell_{u_1} < b_{u_1}$ and $\ell_{u_2} > 0$ hold. Consequently, $x_{u_2}^{\succcurlyeq_{\mathrm{r}}} = 1$ and

$$\sum_{v \in V_+^{\mathrm{r}}(o,u_2) \setminus \{u_2\}} (b_v - \ell_v) > 0$$

holds. Thus, $f_3(\ell, x^{\succcurlyeq_{\mathrm{r}}}) > 0$.

If ℓ satisfies Property (c), then we set $x_u^{\succcurlyeq_{\mathrm{r}}} = 0$ for all $u \in V_+^{\mathrm{r}}(s_1^r, w) \setminus \{s_1^r\}$, otherwise we set $x_u^{\succcurlyeq_{\mathrm{r}}} = 1$. Furthermore, for $i \in V_+^{\mathrm{r}}(o, s_1^r)$,

$$\sum_{v \in V_+^{\mathrm{r}}(o,i) \setminus \{i\}} (b_v - \ell_v) = 0$$

holds due to Property (c). Consequently, $f_3(\ell, x^{\succcurlyeq_{\mathrm{r}}}) = 0$. ∎

Proof of Lemma 20. Let z be feasible for (17). For $i, j \in V_-^{\mathrm{r}}(o, w)$ where $i \preccurlyeq_{\mathrm{r}} j$

$$y_i^{\preccurlyeq_{\mathrm{r}}} y_j^{\succcurlyeq_{\mathrm{r}}} \sum_{v \in V_-^{\mathrm{r}}(i,j) \setminus \{i,j\}} (b_v - \ell_v) \geq 0$$

holds. Assume now that Property (d) does not hold. Consequently, there are $u_1, u_2, u_3 \in V^{\mathrm{r}}_-(o,w) \setminus \{w\}$ with $u_1 \prec_{\mathrm{r}} u_2 \prec_{\mathrm{r}} u_3$ such that $\ell_{u_1} > 0, \ell_{u_2} < b_{u_2}$, and $\ell_{u_3} > 0$ hold. Thus, $y_{u_1}^{\preccurlyeq_{\mathrm{r}}} = y_{u_3}^{\succcurlyeq_{\mathrm{r}}} = 1$ and

$$\sum_{v \in V^{\mathrm{r}}_-(u_1,u_3))\setminus\{u_1,u_3\}} (b_v - \ell_v) > 0$$

holds. Thus, $f_4(\ell, y^{\preccurlyeq_{\mathrm{r}}}, y^{\succcurlyeq_{\mathrm{r}}}) > 0$.

If ℓ satisfies Property (d), then we set $y_v^{\preccurlyeq_{\mathrm{r}}} = 0$ for all $v \in V^{\mathrm{r}}_-(o, t_1^r)\setminus\{t_1^r\}$, otherwise we set $y_v^{\preccurlyeq_{\mathrm{r}}} = 1$. Additionally, we set $y_v^{\succcurlyeq_{\mathrm{r}}} = 1$ for all $v \in V^{\mathrm{r}}_-(o, t_2^r)$ and otherwise we set $y_v^{\succcurlyeq_{\mathrm{r}}} = 0$. Consequently, for $i \in V^{\mathrm{r}}_-(o, t_1^r)\setminus\{t_1^r\}$ or $j \in V^{\mathrm{r}}_-(t_2^r, w)\setminus\{t_2^r\}$, the equality $y_i^{\preccurlyeq_{\mathrm{r}}} y_j^{\succcurlyeq_{\mathrm{r}}} = 0$ holds and for $i, j \in V^{\mathrm{r}}_-(t_1^r, t_2^r)$,

$$\sum_{v \in V^{\mathrm{r}}_-(i,j)\setminus\{i,j\}} (b_v - \ell_v) = 0$$

holds due to Property (d). Consequently, $f_4(\ell, y^{\preccurlyeq_{\mathrm{r}}}, y^{\succcurlyeq_{\mathrm{r}}}) = 0$. ■

Proof of Lemma 23. Optimality of z and the choice of u_1 imply $x_u^{\succcurlyeq_{\mathrm{r}}} = 0$ for all $u \in V^{\mathrm{r}}_+(u_1, w)\setminus\{u_1\}$. Hence,

$$x_i^{\succcurlyeq_{\mathrm{r}}} \sum_{v \in V^{\mathrm{r}}_+(o,i)\setminus\{i\}} (b_v - \ell_v) = 0,$$

whenever $u_1 \in V^{\mathrm{r}}_+(o,i)\setminus\{i\}$. Thus, a change of ℓ_{u_1} does not change $f_3(\ell, x^{\succcurlyeq_{\mathrm{r}}})$. ■

Proof of Lemma 24. Optimality of z and the choice of v_1 and v_3 imply $y_u^{\preccurlyeq_{\mathrm{r}}} = 0$ for all $u \in V^{\mathrm{r}}_-(o, v_1)\setminus\{o, v_1\}$ and $y_u^{\succcurlyeq_{\mathrm{r}}} = 0$ for all $u \in V^{\mathrm{r}}_-(v_3, w)\setminus\{v_3, w\}$. Hence,

$$y_i^{\preccurlyeq_{\mathrm{r}}} y_j^{\succcurlyeq_{\mathrm{r}}} \sum_{v \in V^{\mathrm{r}}_-(i,j)\setminus\{i,j\}} (b_v - \ell_v) = 0,$$

whenever v_1 or v_3 are in $V^{\mathrm{r}}_-(i,j)\setminus\{i,j\}$. Consequently, a change of ℓ_{v_1} or ℓ_{v_3} does not change $f_4(\ell, y^{\preccurlyeq_{\mathrm{r}}}, y^{\succcurlyeq_{\mathrm{r}}})$. ■

Proof of Lemma 27. Let z be an optimal solution of (17). By contradiction, we assume that $f_3(\ell, x^{\succcurlyeq_{\mathrm{r}}}) > 0$ holds. Lemma 19 implies that ℓ does not satisfy Property (c). Consequently, there are entries $u_1, u_2 \in V^{\mathrm{r}}_+(o, w)$ with $u_1 \prec_{\mathrm{r}} u_2$, $\ell_{u_1} < b_{u_1}$, and $\ell_{u_2} > 0$. We now choose u_1 such that $\ell_u = b_u$ holds for all $u \in V^{\mathrm{r}}_+(o, u_1)\setminus\{u_1\}$ and u_2 such that $\ell_u = 0$ holds for all $u \in V^{\mathrm{r}}_+(u_2, w)\setminus\{u_2\}$. Due to the latter, there is an exit $v_2 \in V^{\mathrm{r}}_-(u_2, w)$ with $\ell_{v_2} > 0$ and $\ell_v = 0$ for all $v \in V^{\mathrm{r}}_-(v_2, w)\setminus\{v_2, w\}$. Furthermore, we can assume w.l.o.g. that in a flow decomposition, see Lemma 2, $q(P^{\mathrm{r}}(u_2, v_2)) > 0$ holds. Due to Lemma 4 and $u_1 \prec_{\mathrm{r}} u_2$, we can decrease $q(P^{\mathrm{r}}(u_2, v_2))$ and increase $q(P^{\mathrm{r}}(u_1, v_2))$ such that $\Pi_{P^{\mathrm{r}}(o,w)}(q)$ stays the same as before the modification and $0 < \ell_{u_1} \le b_{u_1}, \ell_{u_2} > 0, \ell_{v_2} > 0$ hold. Thus, the binary variables of z stay the same. Furthermore, by Lemmas 21, 22, and 24 the values of f_1, f_2, and f_4 stay the same. The modified solution satisfies Constraints (17b). The modification only decreases q_a for $a \in P^{\mathrm{r}}(u_2, v_2)$, increases q_a for $a \in P^{\mathrm{r}}(u_1, u_2)$, and the remaining arc flows stay the same. Hence, since $u_1 \prec_{\mathrm{r}} u_2 \prec_{\mathrm{r}} v_2$ and by Lemma 4(d), Constraint (17d) is still satisfied. Consequently, z is still feasible for (17). Due to this modification, we increase $\ell_{u_1} > 0$ and decrease ℓ_{u_2}. By Lemma 23, considering only the decrease of ℓ_{u_2} does not change the objective value. In contrast, the increase of ℓ_{u_1} decreases f_3 because

$$x_{u_2}^{\succcurlyeq_{\mathrm{r}}} \sum_{v \in V^{\mathrm{r}}_+(o,u_2)\setminus\{u_2\}} (b_v - \ell_v)$$

decreases. Thus, the modification decreases the objective value, which is a contradiction to the optimality of the original solution. ■

Proof of Lemma 28. Let z be an optimal solution of (17). By contradiction, we assume that $f_4(\ell, y^{\preccurlyeq_{\mathrm{r}}}, y^{\succcurlyeq_{\mathrm{r}}}) > 0$ holds. Lemma 20 implies that ℓ does not satisfy Property (d). Consequently, there are exits $v_1, v_2, v_3 \in V^{\mathrm{r}}_-(o, w)\setminus\{w\}$ with $v_1 \prec_{\mathrm{r}} v_2 \prec_{\mathrm{r}} v_3$, $\ell_{v_1} > 0, \ell_{v_2} < b_{v_2}$, and $\ell_{v_3} > 0$. Furthermore, we choose v_1 such that $\ell_v = 0$ holds for all $v \in V^{\mathrm{r}}_-(o, v_1)\setminus\{v_1\}$. If $q_a > 0$ for $a \in \delta^{\mathrm{in}}(w) \cap P^{\mathrm{r}}(o, w)$, we replace $v_3 = w$. Otherwise, we choose $v_3 \neq w$ such that $\ell_v = 0$ holds for all $v \in V^{\mathrm{r}}_-(v_3, w)\setminus\{v_3, w\}$. We now consider a flow decomposition such as in Lemma 2. Due to $q \ge 0$, there is an entry $u_3 \in V^{\mathrm{r}}_+(o, v_3)$ with $\ell_u = 0$ for all $u \in V^{\mathrm{r}}_+(u_3, w)\setminus\{u_3\}$ and $q(P^{\mathrm{r}}(u_3, v_3)) > 0$. Furthermore, an entry $u_1 \in V^{\mathrm{r}}_+(o, w)$ with $\ell_u = 0$ for all $u \in V^{\mathrm{r}}_+(o, u_1)\setminus\{o, u_1\}$ exists which satisfies $q(P^{\mathrm{r}}(u_1, v_1)) > 0$. We now distinguish two cases.

Case 1: $v_2 \prec_{\mathrm{r}} u_3$ holds. We now decrease $q(P^{\mathrm{r}}(u_1, v_1))$ by $\varepsilon > 0$ and increase $q(P^{\mathrm{r}}(u_1, v_2))$ by the same amount ε. This increases the potential difference $\Pi_{P(o,w)}(q)$. Thus, we decrease $q(P^{\mathrm{r}}(u_3, v_3))$ by $\tilde{\varepsilon} > 0$. Due to Lemma 4, we can choose ε and $\tilde{\varepsilon}$ such that $\Pi_{P(o,w)}(q)$ stays the same and $\ell_{v_1} > 0, 0 < \ell_{v_2} \le b_{v_2}, \ell_{u_3} > 0, \ell_{v_3} > 0$ hold. Thus, the binary variables of z stay the same. Furthermore, by Lemmas 21–23, the values of f_1, f_2, and f_3 stay the same. The modified solution satisfies

Constraints (17b). Furthermore, the modification only decreases q_a for $a \in P^{\mathrm{r}}(u_3, v_3)$, increases q_a for $a \in P^{\mathrm{r}}(v_1, v_2)$, and the remaining arc flows stay the same. Hence, since $v_1 \prec_{\mathrm{r}} v_2 \prec_{\mathrm{r}} u_3 \prec_{\mathrm{r}} v_3$ and by Lemma 4(d), Constraint (17d) is still satisfied. Consequently, z is still feasible for (17). Due to this modification, we decrease $\ell_{v_1} > 0$ and $\ell_{v_3} > 0$ and increase ℓ_{v_2}. By Lemma 24, considering only the decrease of ℓ_{v_1} and ℓ_{v_3} does not change the objective value. In contrast, the increase of ℓ_{v_2} decreases f_4 because

$$y_{v_1}^{\preccurlyeq_{\mathrm{r}}} y_{v_3}^{\succcurlyeq_{\mathrm{r}}} \sum_{v \in V_{-}^{\mathrm{r}}(v_1, v_3) \setminus \{v_1, v_3\}} (b_v - \ell_v)$$

decreases. Thus, the modification decreases the objective value, which contradicts the optimality of the original solution.
Case 2: $u_3 \prec_{\mathrm{r}} v_2$ holds. We now decrease $q(P^{\mathrm{r}}(u_3, v_3))$ by $\varepsilon > 0$ and increase $q(P^{\mathrm{r}}(u_3, v_2))$ by the same amount ε. This decreases the potential difference $\Pi_{P^{\mathrm{r}}(o,w)}(q)$. Thus, we decrease $q(P^{\mathrm{r}}(u_1, v_1))$ by $\tilde{\varepsilon} > 0$ and increase $q(P^{\mathrm{r}}(u_1, v_2))$ by the same amount $\tilde{\varepsilon}$ which increases the potential difference $\Pi_{P^{\mathrm{r}}(o,w)}(q)$. Due to Lemma 4, we can choose ε and $\tilde{\varepsilon}$ such that $\Pi_{P^{\mathrm{r}}(o,w)}(q)$ stays the same and $\ell_{v_1} > 0, 0 < \ell_{v_2} \leq b_{v_2}, \ell_{v_3} > 0$ hold. In particular, the binary variables of z stay the same. Furthermore, by Lemmas 21–23, the values of f_1, f_2, and f_3 stay the same. The modified solution satisfies Constraints (17b). Furthermore, the modification only decreases q_a for $a \in P^{\mathrm{r}}(v_2, v_3)$, increases q_a for $a \in P^{\mathrm{r}}(v_1, v_2)$, and the remaining arc flows stay the same. Hence, since $v_1 \prec_{\mathrm{r}} v_2 \prec_{\mathrm{r}} v_3$ and by Lemma 4(d), Constraint (17d) is still satisfied.

Consequently, z is still feasible for (17). In analogy to Case 1, the modification decreases f_4, which contradicts the optimality of the original solution. ■

Article 4

Deciding the Feasibility of a Booking in the European Gas Market is coNP-hard

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Deciding the Feasibility of a Booking in the European Gas Market is coNP-hard

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Abstract. We show that deciding the feasibility of a booking (FB) in the European entry-exit gas market is coNP-hard if a nonlinear potential-based flow model is used. The feasibility of a booking can be characterized by polynomially many load flow scenarios with maximum potential-difference, which are computed by solving nonlinear potential-based flow models. We use this existing characterization of the literature to prove that FB is coNP-hard by reducing Partition to the infeasibility of a booking. We further prove that computing a potential-difference maximizing load flow scenario is NP-hard even if we can determine the flow direction a priori. From the literature, it is known that FB can be decided in polynomial time on trees and a single cycle. Thus, our hardness result draws the first line that separates the easy from the hard variants of FB and finally answers that FB is hard in general.

1. Introduction

The entry-exit market system has been introduced for the European gas market as the outcome of the European gas market liberalization [30–32]. One of the main goals of the entry-exit system is to decouple the trade and transport of gas. To this end, the current market system is split into different stages, which are formally described in [19] by a multilevel model of the European entry-exit gas market. In these stages, the transmission system operator (TSO) and the gas traders interact with each other via so-called bookings and nominations. A booking is a mid- to long-term capacity-right contract between the gas traders and the TSO in which the gas traders buy capacity rights for the maximum injection or withdrawal quantity of gas at entry and exit nodes of the network. On a day-ahead basis, the traders nominate the quantity of gas for an injection, respectively withdrawal, on the next day such that the nominated quantity of gas stays within the booked capacities and the total injection and withdrawal quantities are balanced. By signing the booking contracts, the TSO is obliged to guarantee the feasibility of transport of the nominated amounts of gas through the network. Since the gas traders can nominate any booking-compliant nomination, i.e., any balanced quantities of injections and withdrawals up to the booked-capacities, the TSO has to guarantee the feasibility of transport for every booking-compliant nomination. Hence, the TSO has to generally verify the feasibility of infinitely many booking-compliant nominations before the TSO signs a booking. On the one hand, this property of the entry-exit market system decouples trade and transport. On the other hand, it leads to many new

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challenges, e.g., deciding the feasibility of a booking or the computation of bookable capacities, so-called technical capacities; see [9, 25, 28, 37].

In this work, we focus on deciding the feasibility of a booking in general graphs. To this end, we consider passive networks without active elements, i.e., no controllable elements such as valves or compressors are present in the network. We further focus on stationary models of gas transport with nonlinear potential-based flows; see, e.g., [20, 25, 38]. In contrast to the frequently used capacitated linear flows, these physically more accurate potential-based flow models provide additional structure that can be used to decide the feasibility of nominations and bookings. For example, in a passive potential-based flow model, no cyclic flows are possible, which is not necessarily the case for capacitated linear flows. However, the link between node potentials and arc flows is usually given by nonlinear constraints. Consequently, potential-based flows generally lead to a harder class of optimization problems compared to capacitated linear flows. We note that potential-based flows are also used to model hydrogen, water, or power distribution networks; see [20, 35].

Many optimization methods for the transport of gas in pipeline networks have been researched in the recent years, e.g., see the book [24] and the survey article [33] for a comprehensive overview. In doing so, the research mainly focuses on cost-optimal transport, respectively feasible transport, of a single nomination, respectively load flow scenario. The gas flow in pipelines follows physical laws, which lead to challenging mathematical optimization models. Thus, in the literature, approximations considering different classes of optimization models are used. Based on the descriptions in [25, 26, 37], we now state some examples for these approximations. In [7], the gas physics are approximated by piecewise linear functions and the authors analyze the cost-optimal transport in the Belgian network before the European market liberalization. In [3], the cost-optimal transport in the Belgian network is again analyzed considering the different market situation due to the progressed market liberalization. A combination of piecewise linearizations together with sequential quadratic programming is applied in [8]. Furthermore, in many works piecewise linear relaxations are considered for approximating the gas transport, e.g., see [12–15]. Approaches based on continuous nonlinear optimization methods, respectively complementarity-constraint modeling, are used in, e.g., [4, 36, 39–42]. Even more sophisticated and challenging nonlinear mixed-integer models are studied, e.g., in [14, 15, 23]. For details on optimization w.r.t. partial differential equations and optimal control of gas networks, we refer to the survey [21] and the references therein.

Regarding the complexity, deciding the feasibility of a nomination for a linear capacitated flow model as well as for linear potential-based flows is in P since both problems can be decided by solving linear programs; see e.g., [25, 38]. If active elements such as valves are present in the network, then deciding the feasibility of a nomination is NP-hard for the potential-based flow model; see [43].

The literature on bookings, especially on deciding the feasibility of a booking, is rather small in comparison with the research on nominations. Following the literature review in [37], we now briefly summarize the literature on bookings. We note that deciding the feasibility of a booking can be seen as a specific two-stage or adjustable robust feasibility problem, see e.g., [5, 17], since a feasible booking requires the feasibility of all, generally infinitely many, nominations within the given booking bounds. One of the first results about the mathematical properties of bookings are given within the PhD theses [22, 44]. Further structural properties such as (non-)convexity of the set of feasible nominations and bookings are shown in [38]. We note that the reservation-allocation problem considered in [10] is similar to the feasibility of a booking. Moreover, the authors of [2] develop approaches to decide robust feasibility and infeasibility of specific two-stage robust optimization problems using techniques of polynomial optimization. These approaches can also be used to decide the feasibility of a booking in pipe-only networks. In case of capacitated linear flows, deciding the feasibility of a booking is coNP-complete in cyclic networks, but can be decided in polynomial time in tree-shaped networks; see [22]. For the more accurate potential-based flows in pipe-only networks, the feasibility of a booking can be characterized by polynomially many nominations with maximum potential-difference; see [25]. Using this characterization, the authors of [25] show that for linear potential-based flows deciding the feasibility of a booking is in P for general graphs. Additionally, they also prove that this holds for nonlinear potential-based flows in tree-shaped networks; see [25]. We note that the latter also follows from [35] under additional assumptions on the potential bounds. Moreover, the authors of [26] extend these results by proving that deciding the feasibility of a booking in a single cycle is in P. In doing so, again special structures of the nominations with maximum potential-difference are exploited. In this paper, we finally answer that deciding the feasibility of a booking is coNP-hard in cyclic graphs. Thus, we draw the first line that separates the easy from the hard variants of deciding the feasibility of a booking.

We finally refer to the topic of computing maximal feasible bookings, which are called technical capacities. These technical capacities are introduced in [28] and first results are obtained in [22, 44]. They can also be seen as a more sophisticated application of the radius of robust feasibility, e.g., see [6, 16, 27]. Regarding the complexity exponential upper bounds for computing technical capacities w.r.t. capacitated linear flows are given in [22]. An extensive complexity analysis is provided in the recent work [37]. The authors prove that computing technical capacities, i.e., maximizing over the set of feasible bookings, is NP-hard for capacitated linear, linear-, and nonlinear-potential based flows even on trees.

Our contribution is the following. We prove that deciding the feasibility of a booking considering a nonlinear potential-based flow model is coNP-hard in cyclic graphs. The proof is obtained by reducing Partition to the infeasibility of a booking. It is the first hardness result for deciding the feasibility of a booking w.r.t. potential-based flows since the latter is in P for linear potential-based flows in general graphs and for nonlinear potential-based flows in trees and a single-cycle network. We further prove that computing a nomination with maximum potential-difference is NP-hard even if we can determine the flow direction a priori. We summarize our contribution w.r.t. bookings together with a review of the results from the literature in Figure 1, which is an adapted version of Figure 3 in Section 6 of [25].

The remainder of this paper is structured as follows. In Section 2, we formally introduce the problem of deciding the feasibility of a booking. Notations and first results, which are necessary for the hardness proof, are stated in Section 3. Afterward, in Section 4 the coNP-hardness of deciding the feasibility of a booking considering a nonlinear potential-based flow model is shown. Finally, we close with a conclusion in Section 5.

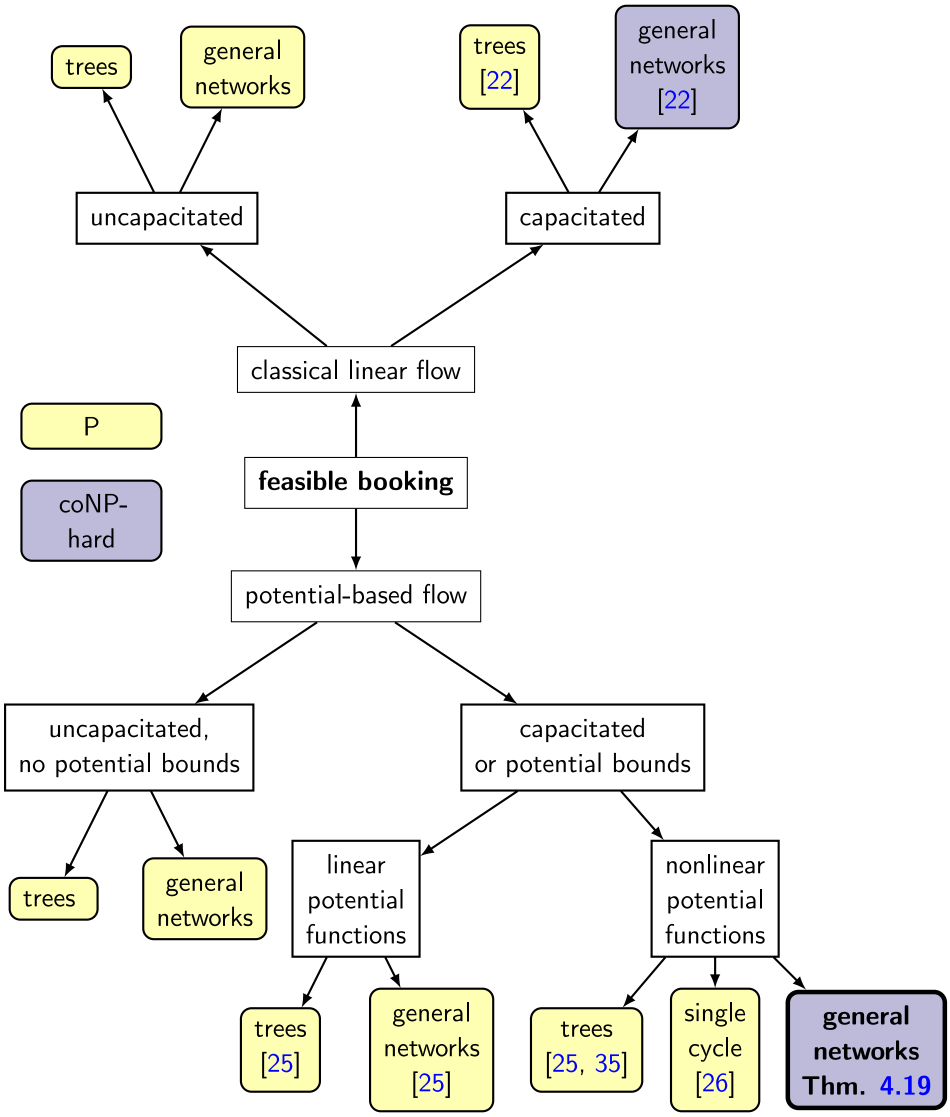

FIGURE 1. Overview of known complexity results for deciding the feasibility of a booking. The figure is an adapted version of the one in Section 6 of [25]. We note that for the case of no flow bounds, respectively no potential bounds, it is not hard to observe that every booking is feasible. Thus, we do not explicitly cite this result.

2. Problem Description

The problem description closely follows the one in [26]. We represent a gas network by a weakly connected and directed graph $G = (V, A)$ with node set V and arc set A. The set of nodes is partitioned into the set V_+ of entry nodes, at which gas is injected, the set V_- of exit nodes, where gas is withdrawn, and the set V_0 of the remaining inner nodes. These node types are equipped with a vector $\sigma = (\sigma_u)_{u \in V}$

given by

$$\sigma_u = \begin{cases} 1, & \text{if } u \in V_+, \\ -1, & \text{if } u \in V_-, \\ 0, & \text{if } u \in V_0. \end{cases}$$

In this paper, only passive networks, i.e., without active elements such as control valves or compressors, are considered. In the following, we introduce notations and definitions which are taken from [26, 38] and follow the corresponding descriptions therein.

Definition 2.1. A *load flow* is a vector $\ell = (\ell_u)_{u\in V} \in \mathbb{R}^V_{\geq 0}$, with $\ell_u = 0$ for all $u \in V_0$. The set of load flow vectors is denoted by L.

A load flow represents an actual situation of the demand in the network at a single point in time by specifying the amount of gas ℓ_u that is injected at $u \in V_+$ or withdrawn at $u \in V_-$. Since we only consider stationary flows, we need to impose that the total injection and withdrawal quantities are balanced, which leads to the definition of a nomination.

Definition 2.2. A *nomination* is a balanced load flow ℓ, i.e., $\sigma^\top \ell = 0$. The set of nominations is given by

$$N := \left\{\ell \in L \colon \sigma^\top \ell = 0\right\}.$$

Definition 2.3. A *booking* is a vector $b = (b_u)_{u\in V} \in \mathbb{R}^V_{\geq 0}$, with $b_u = 0$ for all $u \in V_0$.

Nominations and bookings are linked as described in the following definition.

Definition 2.4. A nomination ℓ is called *booking-compliant* w.r.t. the booking b if $\ell \leq b$ holds, where "$\leq$" is meant component-wise. The set of booking-compliant (or b-compliant) nominations is given by

$$N(b) := \{\ell \in N \colon \ell \leq b\}.$$

As in [26], we now introduce the notion of feasible nominations and bookings. To do so, we model stationary gas flows by an abstract physics model that is based on the Weymouth pressure drop equation and potential-based flows; see, e.g., [20] or [25]. It consists of arc flow variables $q = (q_a)_{a\in A} \in \mathbb{R}^A$ and nodal potentials $\pi = (\pi_u)_{u\in V} \in \mathbb{R}^V_{\geq 0}$. These arc flows couple the potentials, which leads to the nonlinear potential-based flow model (1). We note that in gas networks with horizontal pipes the potentials π are closely linked to the gas pressures p at the nodes of the pipeline networks by $\pi_u = p_u^2$ for $u \in V$. In case of non-horizontal pipes, we refer to [24].

Definition 2.5. A nomination $\ell \in N$ is *feasible* if a point (q, π) exists that satisfies

$$\sum_{a\in\delta^{\text{out}}(u)} q_a - \sum_{a\in\delta^{\text{in}}(u)} q_a = \sigma_u \ell_u, \qquad u \in V, \tag{1a}$$

$$\pi_u - \pi_v = \Lambda_a q_a \left|q_a\right|, \qquad a = (u, v) \in A, \tag{1b}$$

$$\pi_u \in [\pi_u^-, \pi_u^+], \qquad u \in V, \tag{1c}$$

where $\delta^{\text{out}}(u)$ and $\delta^{\text{in}}(u)$ represent the set of arcs leaving and entering node $u \in V$, $\Lambda_a > 0$ is an arc-specific constant for any $a \in A$, and $0 < \pi_u^- \le \pi_u^+$ are potential bounds for any $u \in V$.

Constraints (1a) ensure mass flow conservation at every node of the network. The flows q couple the potentials for every arc of the network in Constraint (1b). Since we model a gas network as a directed graph, we can interpret the direction of flow. Thus, for an arc $(u, v) \in A$, the arc flow can be negative if it flows in the opposite direction of the orientation of the arc, i.e., if it flows from v to u. Moreover, technical restrictions of the network impose that the potentials are bounded (1c). For other models of gas transport such as capacitated linear and linear potential-based flows, we refer to [25, 38].

For a given nomination $\ell \in N$ and a weakly connected pipe-only network, the corresponding flows $q = q(\ell)$, i.e., they satisfy Constraints (1a) and (1b), are unique because they are the optimal solution of a strictly convex minimization problem; see [29]. Moreover, the corresponding potentials $\pi = \pi(\ell)$ are unique up to constant shifts; see [34]. Consequently, the potential differences $\pi_u - \pi_v$ for $u, v \in V$ are unique for a given nomination ℓ. We further note that the feasibility of a nomination can be verified by different approaches; see e.g., [18, 24]. We now turn to the feasibility of a booking, which is less studied in the literature and very challenging.

Definition 2.6. We say that a booking b is *feasible* if all booking-compliant nominations $\ell \in N(b)$ are feasible.

For deciding the feasibility of a booking, an infinite number of nominations has to be checked for feasibility, in general. As in [26], we make the following non-restrictive assumption on the potential bounds.

Assumption 2.7. The potential bound intervals have a non-empty intersection, i.e.,

$$\bigcap_{u \in V} [\pi_u^-, \pi_u^+] \neq \emptyset.$$

This assumption is a necessary condition for the feasibility of a booking, since it ensures that the zero nomination, which is always booking-compliant, with corresponding zero flows is feasible in the network. Consequently, from the infeasibility of this assumption, it directly follows that all bookings are infeasible. Moreover, we can check this assumption in polynomial time a priori.

It is shown in [25], that the feasibility of a booking b can be characterized by polynomially many nominations with maximum potential-difference between all pairs of nodes. To this end, the authors introduce, for every fixed pair of nodes $(w_1, w_2) \in V^2$, the following problem

$$\begin{aligned} \varphi_{w_1 w_2}(b) := \max_{\ell, q, \pi} \quad & \pi_{w_1} - \pi_{w_2} && \text{(2a)} \\ \text{s.t.} \quad & 0 \le \ell_u \le b_u, \quad u \in V, && \text{(2b)} \\ & \text{(1a)}, \text{(1b)}, \end{aligned}$$

where $\varphi_{w_1 w_2}$ is the corresponding optimal value function that depends on the booking b. Problem (2) computes the maximum potential difference between the given nodes w_1 and w_2. We note that the zero vector is feasible for Problem (2) due to Assumption 2.7. Consequently, an optimal solution always exists since the variables ℓ and q are bounded, and thus, we can bound the potentials π by a finite positive constant due to Theorem 7.1 of Chapter 7 in [24]. From Theorem 10 in [25] it follows that booking b is feasible if and only if

$$\varphi_{w_1 w_2}(b) \le \pi_{w_1}^{+} - \pi_{w_2}^{-}$$

holds for every fixed pair of nodes $(w_1, w_2) \in V^2$. Exploiting this approach, we can decide the feasibility of a booking by solving the nonlinear and nonconvex optimization problems (2) for every pair of nodes. For trees and single-cycle networks, this can be done in polynomial time; see [25, 26, 35]. In this paper, we show that deciding the feasibility of a booking w.r.t. nonlinear potential-based flow model (1) is coNP-hard. We further prove that the decision variant of (2) is NP-hard. To this end, we formally define the problem of deciding the feasibility of a booking w.r.t. nonlinear potential-based flow model (1) and the decision problem corresponding to (2).

Deciding the Feasibility of a Booking (FB).

Input:	Graph $G = (V, A)$ with entries V_+, exits V_-, inner nodes V_0, potential drop coefficients $\Lambda_a \in \mathbb{Q}_{>0}$ for $a \in A$, potential bounds $\pi_u^- \le \pi_u^+, \pi_u^-, \pi_u^+ \in \mathbb{Q}_{>0}$ for all $u \in V$, and a booking $b \in \mathbb{Q}_{\ge 0}^{V}$.
Question:	Is booking b feasible, i.e., does for every booking-compliant nomination $\ell \in N(b)$ a feasible point (q, π) for (1) exist?

Computing a Maximum Potential-Difference Nomination (MPD).

Input:	Graph $G = (V, A)$ with entries V_+, exits V_-, inner nodes V_0, potential drop coefficients $\Lambda_a \in \mathbb{Q}_{>0}$ for $a \in A$, a booking $b \in \mathbb{Q}_{\ge 0}^{V}$, two nodes $w_1, w_2 \in V$, and a threshold $T \in \mathbb{Q}$.
Question:	Does a solution of (2) with objective $\varphi_{w_1 w_2}(b) \ge T$ exist?

3. Notations and Basic Observations

We now introduce notations and basic observations, which are taken from [26]. Using these results, we prove that FB w.r.t. our nonlinear potential-based flow model (1) is coNP-hard in Section 4. In the following, we consider the directed and weakly connected graph $G = (V, A)$ that models the considered gas network. For a nomination $\ell \in N$, entry and exit nodes $v \in V_+ \cup V_-$ are called *active* if $\ell_v > 0$ holds. We denote the set of active entries by $V_+^{>} := \{v \in V_+ : \ell_v > 0\}$ and the set of active exits by $V_-^{>} := \{v \in V_- : \ell_v > 0\}$. Furthermore, the set of non-zero nominations is given by $N^0 := N \setminus \{0\}$.

Modeling gas networks by directed graphs enables us to interpret the direction of arc flows. However, the physical flow in a potential-based network is independent from the direction of the arcs. Thus, exactly as in [26], we introduce so-called *flow-paths*. For nodes $u, v \in V$, a flow-path $P(u, v) = (V(P(u, v)), A(P(u, v)))$ consists of the set of nodes $V(P(u, v)) \subseteq V$ that contains the nodes of a path from u to v in the undirected graph underlying G and the set of arcs $A(P(u, v)) \subseteq A$ contains the corresponding arcs of this path. We call $P(u, v)$ a directed flow-path from u to v if $P(u, v)$ is a directed path from u to v in G. For another pair of nodes $u', v' \in V$, we denote $P(u', v')$ as a *flow-subpath* of $P(u, v)$ if $P(u', v') \subseteq P(u, v)$, i.e., $V(P(u',v')) \subseteq V(P(u,v))$ and $A(P(u',v')) \subseteq A(P(u,v))$ hold, and if $P(u',v')$ is itself a flow-path. If it is clear from the context, we use the simplified notation $u \in P = P(u,v)$ instead of $u \in V(P(u,v))$ or $a \in P$ instead of $a \in A(P(u,v))$ in the following. Additionally, we introduce an order on the nodes of a flow-path as in [26]. For $P = P(u,v)$ and $u', v' \in P$, we define $u' \preceq_P v'$ if and only if flow-subpaths $P(u,u') \subseteq P(u,v')$ exist. If $u' \neq v'$ holds, we write $u' \prec_P v'$. We note that the considered flow-paths do not contain any cycles in the graph underlying G. This is in line with the considered physics of gas transport, since in every solution (q,π) of (1) no cyclic flow exists due to (1b).

For an arc $a = (u,v) \in A$, we now introduce the following *characteristic function*

$$\chi_a(P) := \begin{cases} 1, & \text{if } u \prec_P v, \\ -1, & \text{if } v \prec_P u, \\ 0, & \text{if } a \notin P, \end{cases}$$

where P is an arbitrary flow-path. The following lemma of [26] uses a classical result from linear flow models to construct a flow decomposition without cyclic flows.

Lemma 3.1 (Lemma 2 in [26])**.** For $\ell \in N^0$, let $\mathcal{P}_\ell := \left\{P(u,v) \colon u \in V_+^>, v \in V_-^>\right\}$ be the set of flow-paths in G with an active entry as start node and an active exit as end node. Then, a decomposition of the given arc flows $q = q(\ell)$, satisfying (1a) and (1b), into path flows exists, such that

$$q_a = \sum_{P \in \mathcal{P}_\ell} \chi_a(P)\, q(P), \quad a \in A,$$

where $q(P)$ is the nonnegative flow along the flow-path $P \in \mathcal{P}_\ell$.

Furthermore, we require that if $q_a > 0$ for $a \in A$ and $\chi_a(P) = -1$ for $P \in \mathcal{P}_\ell$, then $q(P) = 0$ holds. Similarly, if $q_a < 0$ for $a \in A$ and $\chi_a(P) = 1$ for $P \in \mathcal{P}_\ell$, then $q(P) = 0$ holds.

We also observe as in [26], that we can express a nomination by the constructed flow-paths.

Corollary 3.2 (Corollary 3 in [26])**.** For any $u \in V_+^>$, the condition

$$\sum_{v \in V_-^>} q(P(u,v)) = \ell_u$$

and for any $v \in V_-^>$, the condition

$$\sum_{u \in V_+^>} q(P(u,v)) = \ell_v$$

is satisfied.

Exactly as in [26], we can express the potential-difference function along a given flow-path.

Definition 3.3. Let $\ell \in N$ and a flow-path P be given. Then, the *potential-difference function* along P is given by

$$\Pi_P : \mathbb{R}^A \to \mathbb{R}, \quad \Pi_P(q) := \sum_{a \in P} \chi_a(P) \Lambda_a q_a \left|q_a\right|,$$

with $q = q(\ell)$.

As described in [26], from Constraints (1b) it follows that for any node pair $u, v \in V$ and for any flow-path $P := P(u, v)$, the equation $\pi_u(\ell) - \pi_v(\ell) = \Pi_P(q(\ell))$ is satisfied. If P is a directed flow-path from u to v, then the potential-difference function simplifies to

$$\Pi_P(q) = \sum_{a \in P} \Lambda_a q_a |q_a| .$$

As last basic observation, we explicitly state some properties for directed flow-paths and the potential-difference function proven in [26].

Lemma 3.4 (Lemma 4 in [26])**.** For $u, v \in V$, let $P := P(u, v)$ be a directed flow-path from u to v. Then, the following holds:

(a) Π_P is continuous.
(b) Π_P is strictly increasing w.r.t. every component. That means, for q fixed except for one value q_a, $a \in P$, Π_P is increasing in q_a.
(c) Π_P is unbounded w.r.t. every component, i.e., for $a \in P$,

$$\lim_{q_a \to -\infty} \Pi_P = -\infty \quad \text{and} \quad \lim_{q_a \to \infty} \Pi_P = \infty.$$

(d) Π_P is additive w.r.t. the flow-path, i.e., for all $v' \in P$,

$$\Pi_P = \Pi_{P(u,v')} + \Pi_{P(v',v)}$$

with $P = P(u, v') \cup P(v', v)$.
(e) $\Pi_P \geq 0$ holds if and only if $\pi_u \geq \pi_v$ holds.

4. Hardness

In this section, we prove that deciding the feasibility of a booking (FB) w.r.t. nonlinear potential-based flow model (1) is coNP-hard. To this end, we reduce Partition to the infeasibility of a booking. We consider Partition as it is defined in [11] with the small adaption that $n \geq 3$ holds. We note that this variant of Partition is still NP-hard; see [11].

Partition (Part).
Input: $S_1, \dots, S_n \in \mathbb{N}$ with $n \geq 3$, $I = \{1, \dots, n\}$, and $\sum_{i \in I} S_i = K$.
Question: Does $I_1 \subseteq I$ with $\sum_{i \in I_1} S_i = \sum_{I \setminus I_1} S_i$ exist?

For a given Partition instance, we now construct a corresponding booking instance with its graph $G(\mathsf{Part}) = (V, A)$. To this end, we introduce for every number S_i of the given Partition instance an entry node z_i^+ and an exit node z_i^-, which are connected by an arc. Furthermore, we add a main entry node o and a main exit node w. Each of these two nodes is connected to every entry node z_i^+ for $i \in I$. The booking and potential bounds are chosen such that we only have to consider (2) w.r.t. (o, w) for deciding the feasibility of the considered booking. We then prove that the corresponding objective value, i.e., the potential-difference between o and w, exceeds a certain threshold value if and only if Partition is feasible. In detail, graph $G(\mathsf{Part}) = (V, A)$ is constructed as

$$V_+ = \{o, z_1^+, \dots, z_n^+\}, \quad V_- = \{w, z_1^-, \dots, z_n^-\}, \quad V = V_+ \cup V_-,$$
$$A = \{(o, z_i^+) : i \in I\} \cup \{(z_i^+, z_i^-) : i \in I\} \cup \{(z_i^+, w) : i \in I\} .$$

A visualization of the graph $G(\mathsf{Part})$ is given in Figure 2. We consider for $G(\mathsf{Part})$

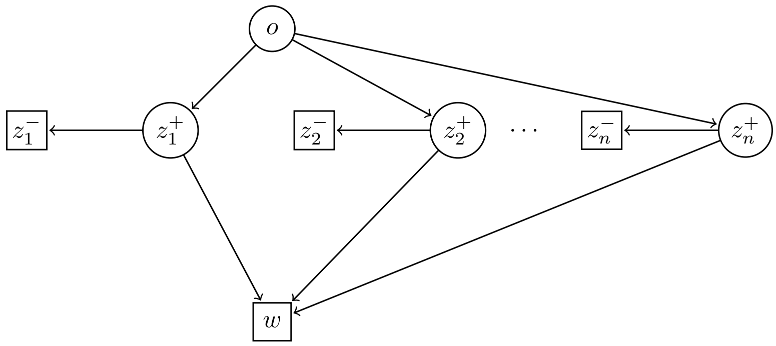

FIGURE 2. The graph $G(\mathsf{Part})$. Entry nodes are indicated by circles and exit nodes by boxes

the booking b

$$b_o = b_w = \frac{K}{2}, \quad b_{z_i^+} = b_{z_i^-} = S_i, \quad i \in I,$$

and potential drop coefficients $\Lambda_a > 0$ for $a \in A$ given by

$$\Lambda_{(o,z_i^+)} = \Lambda_{(z_i^+,w)} = \frac{1}{S_i^2}, \ \Lambda_{(z_i^+,z_i^-)} = 1, \quad i \in I.$$

We finally set the potential bounds for this booking instance. To this end, we first introduce some parameters depending on the input K that are required throughout this section.

$$\varepsilon(K) = 1 - \left(\frac{K - \frac{1}{8K}}{K}\right)^2, \quad M(K) = \max\left\{1 - \varepsilon(K) + \varepsilon(K)^2, 1 - \frac{\varepsilon(K)^2}{K^2}\right\}, \tag{3a}$$

$$\tilde{\varepsilon}(K) = \frac{1}{5}(1 - M(K)), \qquad T(K) = \max\left\{1 - \frac{\tilde{\varepsilon}(K)^2}{K^2 n^2}, M(K) + 4\tilde{\varepsilon}(K)\right\}. \tag{3b}$$

We note that $0 < T(K) < 1$ holds due to $K \geq 1$. Further, we do not explicitly simplify these parameters by computing the maxima, because each of these parameters is separately used in the following proofs. Thus, the extensive form of (3a) and (3b) is useful for the remainder of this section.

The lower π^- and upper π^+ potential bounds for $G(\mathsf{Part})$ are given by

$$\pi_o^+ = \pi_w^+ = 9K^2 + 1, \quad \pi_u^+ = 18K^2 + 1, \ u \in V \setminus \{o, w\},$$
$$\pi_u^- = 0, \ u \in V \setminus \{w\}, \quad \pi_w^- = \pi_w^+ - T(K).$$

We note that for a given instance of Partition, we can build the corresponding booking instance $G(\mathsf{Part})$ in polynomial time and its coding length is polynomially bounded from above by the coding length of the given Partition instance. We now consider $G(\mathsf{Part})$ and its booking b throughout this section. From Section 2, it follows that the booking b is feasible if and only if

$$\varphi_{w_1 w_2}(b) \leq \pi_{w_1}^+ - \pi_{w_2}^- \tag{4}$$

holds for every fixed pair of nodes $(w_1, w_2) \in V^2$, where $\varphi_{w_1 w_2}(b)$ is the optimal value function of (2) that denotes the maximum potential-difference between w_1 and w_2 within booking b.

We first show that Inequality (4) is directly satisfied for $(w_1, w_2) \in V^2 \setminus \{(o, w)\}$, due to the choice of the lower and upper potential bounds.

Lemma 4.1. For any node pair $(w_1, w_2) \in V^2 \setminus \{(o, w)\}$ of $G(\mathsf{Part}) = (V, A)$, Inequality (4) is satisfied.

Proof. Let (q, π) be an optimal solution of $\varphi_{w_1 w_2}(b)$. We note that for the case $w_1 = w_2$, the equation $\varphi_{w_1 w_2}(b) = 0$ holds and, thus, Condition (4) is satisfied in this case due to $\pi_u^- \leq \pi_u^+$ for all $u \in V$. Consequently, we assume $w_1 \neq w_2 \in V$ in the following. From (1a), (1b), and $\sum_{u \in V_+} b_u = (3/2)K$, it follows $|q_a| \leq (3/2)K$ for every arc $a \in A$. For an arbitrary flow-path $P(w_1, w_2)$, it holds

$$\pi_{w_1} - \pi_{w_2} = \sum_{a \in A(P(w_1, w_2))} \chi_a(P) \Lambda_a q_a |q_a| \leq |A(P(w_1, w_2))| \left(\frac{3}{2}K\right)^2.$$

Since the flow-path $P(w_1, w_2)$ with minimal number of arcs consists of at most 4 arcs, this leads to

$$\pi_{w_1} - \pi_{w_2} \leq 4 \left(\frac{3}{2}K\right)^2 = 9K^2$$

$$< \pi_{w_1}^+ - \pi_{w_2}^- = \begin{cases} 9K^2 + 1, & \text{if } w_1 \in \{o, w\}, w_2 \neq w \\ 18K^2 + 1, & \text{if } w_1 \in V \setminus \{o, w\}, w_2 \neq w \\ 9K^2 + T(K), & \text{if } w_1 \in V \setminus \{o, w\}, w_2 = w. \end{cases}$$

□

Consequently, deciding the feasibility of booking b for $G(\mathsf{Part})$ reduces to the following.

Corollary 4.2. Booking b is feasible for $G(\mathsf{Part})$ if and only if $\varphi_{ow}(b) \leq T(K)$.

In the remainder of this section, we prove that $\varphi_{ow}(b) > T(K)$ is satisfied if and only if the given Partition instance is feasible. From now on, we use Partition is feasible, respectively infeasible, as a short form for the given Partition instance is feasible, respectively infeasible. We first prove that if Partition is feasible, then $\varphi_{ow}(b)$ exceeds the threshold $T(K)$.

Lemma 4.3. If Partition is feasible, then $\varphi_{ow}(b) \geq 1 > T(K)$ holds.

Proof. Since Partition is feasible, $M_1 \subset I$ and $M_2 \subset I$ with $M_1 \cap M_2 = \emptyset$ and $M_1 \cup M_2 = I$ exist such that $\sum_{i \in M_1} S_i = \sum_{i \in M_2} S_i = K/2$ holds. We now construct a feasible point (ℓ, q, π) of (2) w.r.t. (o, w) that has an objective value of 1.

$$\begin{aligned}
&\ell_o = \ell_w = \frac{K}{2}, \quad \ell_{z_i^-} = S_i,\ \ell_{z_i^+} = 0,\ i \in M_1, \quad \ell_{z_i^+} = S_i,\ \ell_{z_i^-} = 0,\ i \in M_2, \\
&q_{(o, z_i^+)} = q_{(z_i^+, z_i^-)} = S_i,\ q_{(z_i^+, w)} = 0,\ i \in M_1, \\
&q_{(o, z_i^+)} = q_{(z_i^+, z_i^-)} = 0,\ q_{(z_i^+, w)} = S_i,\ i \in M_2, \\
&\pi_o = \pi_{z_i^+} = \pi_{z_i^-} = \pi_o^+,\ i \in M_2, \quad \pi_{z_i^+} = \pi_o^+ - 1,\ \pi_{z_i^-} = \pi_{z_i^+} - S_i^2,\ i \in M_1, \\
&\pi_w = \pi_o - 1.
\end{aligned}$$

Since (ℓ, q, π) is a feasible point for (2) w.r.t. (o, w) with objective value of 1, the optimal solution of $\varphi_{ow}(b)$ has an objective value of at least $1 > T(K)$. □

We next prove that if we require nonnegative flow in (2) and Partition is infeasible, then an optimal solution does not exceed the threshold value $T(K)$, i.e., $\varphi_{ow}(b) < T(K)$ holds. To this end, we introduce the nonnegative flow variant of (2) for node pair (o, w):

$$\varphi^+_{ow}(b) := \max_{\ell,q,\pi} \quad \pi_o - \pi_w \tag{5a}$$
$$\text{s.t.} \quad 0 \leq \ell_u \leq b_u, \qquad u \in V, \tag{5b}$$
$$q_a \geq 0, \qquad a \in A, \tag{5c}$$
$$\text{(1a)}, \text{(1b)},$$

where $\varphi^+_{ow}(b)$ is the corresponding optimal value function.

With the help of Lemmas 4.5–4.12, we prove that $\varphi^+_{ow}(b) < T(K)$ is satisfied if Partition is infeasible. Afterward, we use these results to show the general case $\varphi_{ow}(b) < T(K)$. The main idea is that if Partition is infeasible, then for at least one $i \in I$ the flows satisfy $q_{(o,z_i^+)} > 0$ and $q_{(z_i^+,w)} > 0$; see Lemma 4.6. This together with the considered nonlinear potential-based flow (1b) plays an important role in the remaining section which is based on the following observation.

Observation 4.4. Let be $a > 0$ and $b > 0$ with $a^2 + b^2 = c$. Then, $a + b > \sqrt{c}$ holds.

To provide an intuition for the main idea, we give the following explanation. For every $i \in I$ and solution (ℓ, q, π) of (5), the equality

$$\pi_o - \pi_w = \Lambda_{(o,z_i^+)} q^2_{(o,z_i^+)} + \Lambda_{(z_i^+,w)} q^2_{(z_i^+,w)}$$

holds. From Observation 4.4, it follows that we need strictly more flow in terms of $q_{(o,z_i^+)} + q_{(z_i^+,w)}$ to obtain a potential difference of $\pi_o - \pi_w$ if $q_{(o,z_i^+)} > 0$ and $q_{(z_i^+,w)} > 0$ hold in comparison to the case if one of these flows is zero. We prove in Lemma 4.6 that if Partition is infeasible, $q_{(o,z_i^+)} > 0$ and $q_{(z_i^+,w)} > 0$ for at least one $i \in I$ in an optimal solution of (5) is satisfied. The latter is not necessarily the case if Partition is feasible; see Lemma 4.3. Consequently, we need strictly more flow to obtain a certain potential difference $\pi_o - \pi_w$ if Partition is infeasible in contrast to the case if Partition is feasible. This is one of the main reasons why the optimal value of (5) cannot exceed the threshold $T(K)$ if Partition is infeasible due to the monotonicity of the potential drop $\Pi_P(q)$ w.r.t. the flow q; see Lemma 3.4 (b).

We start the proof of $\varphi^+_{ow}(b) < T(K)$ by characterizing optimal solutions of (5) in the next two lemmas.

Lemma 4.5. Let (ℓ, q, π) be an optimal solution of (5). Then,

$$\ell_o = \ell_w = \frac{K}{2} = b_o = b_w$$

holds.

Proof. We consider a flow decomposition of Lemma 3.1 and prove the claim by the distinction of three different cases.

If $\ell_o < K/2$ and $\ell_w < K/2$ hold, then from Lemma 3.4 it follows that $\varepsilon_i > 0$ for all $i \in I$ exist such that

$$\ell_o + \sum_{i \in I} \varepsilon_i \leq \frac{K}{2} = b_o, \quad \ell_w + \sum_{i \in I} \varepsilon_i \leq \frac{K}{2} = b_w$$

and we can increase the flow $q(P_i(o, w))$ by ε_i for $i \in I$, such that the potential drop $\Pi_{P_i(o,w)}$ is the same for $i \in I$. Here, $P_i(o, w)$ is the directed flow-path from o to w via z_i^+, i.e., $P_i(o, w) = (\{o, z_i^+, w\}, \{(o, z_i^+), (z_i^+, w)\})$. The modification increases the potential drop $\pi_o - \pi_w$ due to Lemma 3.4 (b). This is a contradiction to the optimality of (ℓ, q, π) for (5).

If $\ell_o = K/2$ and $\ell_w < K/2$ hold, then from (1a) and (5c) it follows that $i \in I$ exist such that $q(P(o, z_i^-)) > 0$ for $P(o, z_i^-) = (\{o, z_i^+, z_i^-\}, \{(o, z_i^+), (z_i^+, z_i^-)\})$ holds. We additionally consider the flow-path $P_i(o, w)$ as in the above case. Due to Lemma 3.4 and the graph structure of $G(\mathsf{Part})$, $\varepsilon > 0$ and $0 < \tilde{\varepsilon} < \varepsilon$ exist such that decreasing $q(P(o, z_i^-))$ by ε and increasing $q(P_i(o, w))$ by $\tilde{\varepsilon}$ does not change the potential drop $\Pi_{P_i(o,w)}$ and $\ell_w < K/2$ as well as (5c) still holds. Consequently, $\ell_o < K/2$ and $\ell_w < K/2$ is satisfied and in analogy to the above this is a contradiction to the optimality of the considered solution.

If $\ell_w = K/2$ and $\ell_o < K/2$ are satisfied, then from (1a) and (5c) it follows that $i \in I$ exist such that $q(P(z_i^+, w)) > 0$ for $P(z_i^+, w) = (\{z_i^+, w\}, \{(z_i^+, w)\})$ holds. We again consider the flow-path $P_i(o, w)$ as before. Due to Lemma 3.4 and the graph structure of $G(\mathsf{Part})$, $\varepsilon > 0$ and $0 < \tilde{\varepsilon} < \varepsilon$ exist such that decreasing $q(P(z_i^+, w))$ by ε and increasing $q(P_i(o, w))$ by $\tilde{\varepsilon}$ does not change the potential drop $\Pi_{P_i(o,w)}$ and $\ell_o < K/2$ as well as (5c) still holds. Consequently, $\ell_o < K/2$ and $\ell_w < K/2$ is satisfied and in analogy to the above this is a contradiction to the optimality of the considered solution. □

We now show that if Partition is infeasible, then every optimal solution of (5) satisfies that at least one flow-path $P_i(o, w) = (\{o, z_i^+, w\}, \{(o, z_i^+), (z_i^+, w)\})$ with $i \in I$ and $q_a > 0$ for $a \in A(P_i(o, w))$ exists.

Lemma 4.6. If Partition is infeasible, then for any optimal solution (ℓ, q, π) of (5), there exists an index $i \in I$ such that $q_{(o,z_i^+)} > 0$ and $q_{(z_i^+,w)} > 0$ hold.

Proof. We prove the contraposition. To this end, let (ℓ, q, π) be an optimal solution of (5) that satisfies $q_{(o,z_i^+)} = 0$ or $q_{(z_i^+,w)} = 0$ for each $i \in I$. Due to Lemma 4.5 and (5c), $q_{(o,z_i^+)} = q_{(z_i^+,w)} = 0$ is not satisfied for any $i \in I$ in an optimal solution of (5). Thus, the index sets

$$M_1 = \left\{i \in I : q_{(o,z_i^+)} > 0\right\}, \quad M_2 = \left\{i \in I : q_{(z_i^+,w)} > 0\right\}$$

satisfy $M_1 \cap M_2 = \emptyset$ and $M_1 \cup M_2 = I$. Consequently, from (1a), (5b), and (5c), we obtain the flow bounds

$$q_{(o,z_i^+)} \leq S_i, \; q_{(z_i^+,w)} \leq S_i, \quad i \in I. \tag{6}$$

Furthermore, from Lemma 4.5 it follows $\ell_o = \ell_w = K/2$. The latter together with flow conservation (1a) and (6), leads to

$$\frac{K}{2} = \sum_{i \in I} q_{(o,z_i^+)} = \sum_{i \in M_1} q_{(o,z_i^+)} \leq \sum_{i \in M_1} S_i,$$
$$\frac{K}{2} = \sum_{i \in I} q_{(z_i^+,w)} = \sum_{i \in M_2} q_{(z_i^+,w)} \leq \sum_{i \in M_2} S_i.$$

From this and $\sum_{i\in M_1\cup M_2} S_i = \sum_{i\in I} S_i = K$, we obtain

$$\frac{K}{2} = \sum_{i\in M_1} S_i = \sum_{i\in M_2} S_i$$

and thus, Partition is feasible. □

With the help of the previous two lemmas, we now prove that if Partition is infeasible, then the optimal value of (5) is strictly smaller than 1.

Lemma 4.7. If Partition is infeasible, then $\varphi^+_{ow}(b) < 1$ holds.

Proof. Let (ℓ, q, π) be an optimal solution of (5) with objective value ϕ. Due to Lemma 4.5 and flow conservation (1a), the equalities

$$\frac{K}{2} = \sum_{i\in I} q_{(o,z_i^+)}, \quad \frac{K}{2} = \sum_{i\in I} q_{(z_i^+,w)}, \tag{7}$$

are satisfied. From Lemma 4.6, it follows that an index $l \in I$ with $q_{(o,z_l^+)} > 0$ and $q_{(z_l^+,w)} > 0$ exists. The equality $q^2_{(o,z_i^+)} + q^2_{(z_i^+,w)} = \phi S_i^2$ is satisfied for all $i \in I$ due to (1b) and (5c). Applying Observation 4.4 leads to

$$q_{(o,z_l^+)} + q_{(z_l^+,w)} > \sqrt{\phi} S_l, \quad q_{(o,z_i^+)} + q_{(z_i^+,w)} \geq \sqrt{\phi} S_i, \quad i \in I \setminus \{l\}.$$

From this and (7), we obtain

$$\begin{aligned} K &= \sum_{i\in I\setminus\{l\}} \left(q_{(o,z_i^+)} + q_{(z_i^+,w)}\right) + q_{(o,z_l^+)} + q_{(z_l^+,w)} \\ &> \sqrt{\phi} \sum_{i\in I\setminus\{l\}} S_i + \sqrt{\phi} S_l = \sqrt{\phi} K, \end{aligned}$$

which implies $\phi < 1$. □

Up to now, we have shown that if Partition is infeasible, then $\varphi^+_{(o,w)}(b) < 1$ is satisfied. In the following Lemmas 4.8–4.12, we strengthen that result and show that if Partition is infeasible, then $\varphi^+_{(o,w)}(b) < T(K) < 1$ holds, which is essential due to Corollary 4.2. To this end, for a feasible point (ℓ, q, π) of (5) with positive objective value, we introduce the following partition of the indices I

$$M_1 = \left\{ i \in I \colon q_{(o,z_i^+)} > 0, q_{(z_i^+,w)} = 0 \right\}, \tag{8a}$$

$$M_2 = \left\{ i \in I \colon q_{(o,z_i^+)} = 0, q_{(z_i^+,w)} > 0 \right\}, \tag{8b}$$

$$M_3 = \left\{ i \in I \colon q_{(o,z_i^+)} > 0, q_{(z_i^+,w)} > 0 \right\}. \tag{8c}$$

We note that $q_{(o,z_i^+)} = q_{(z_i^+,w)} = 0$ does not hold for any $i \in I$ due to the positive objective value of the considered feasible point (ℓ, q, π). Moreover, the parameters $\varepsilon(K)$ and $M(K)$ of (3a) come now into play.

Lemma 4.8. Let Partition be infeasible. If (ℓ, q, π) is an optimal solution of (5) such that $q_{(o,z_l^+)} > 0$ and $q_{(z_l^+,w)} > 0$ hold for exactly one index $l \in I$, then the corresponding objective value ϕ satisfies

$$\phi < \left(\frac{K - \frac{1}{8K}}{K}\right)^2 = 1 - \varepsilon(K) < 1.$$

Proof. We contrarily assume that an optimal solution (ℓ, q, π) of (5) exists such that the requirements are satisfied and the objective value ϕ satisfies $\phi \geq 1 - \varepsilon(K) > 0$. From Lemma 4.7, it follows $\phi < 1$. We partition the index set I according to (8).

Due to the requirements, $M_1 \cap M_2 = \emptyset$, $M_3 = \{l\}$, and $M_1 \cup M_2 \cup \{l\} = I$ hold. Consequently, Lemma 4.5 and flow conservation (1a) lead to

$$\frac{K}{2} = \sum_{i \in M_1} q_{(o,z_i^+)} + q_{(o,z_l^+)}, \quad \frac{K}{2} = \sum_{i \in M_2} q_{(z_i^+,w)} + q_{(z_l^+,w)}. \tag{9}$$

Additionally,

$$q^2_{(o,z_i^+)} + q^2_{(z_i^+,w)} = \phi S_i^2, \quad i \in I, \tag{10}$$

is satisfied due to (1b) and (5c) and thus, it follows

$$q_{(o,z_i^+)} = \sqrt{\phi} S_i, \ i \in M_1, \quad q_{(z_i^+,w)} = \sqrt{\phi} S_i, \ i \in M_2. \tag{11}$$

This together with (9) leads to

$$q_{(o,z_l^+)} = \frac{K}{2} - \sqrt{\phi} \sum_{i \in M_1} S_i, \quad q_{(z_l^+,w)} = \frac{K}{2} - \sqrt{\phi} \sum_{i \in M_2} S_i. \tag{12}$$

We now distinguish different cases for the value of $\sum_{i \in M_1} S_i$, respectively $\sum_{i \in M_2} S_i$.

If $\sum_{i \in M_1} S_i = K/2$ holds, then $\sum_{i \in I \setminus M_1} S_i = K/2$ holds due to $\sum_{i \in I} S_i = K$. This is a contradiction to the infeasibility of Partition. In analogy it follows that $\sum_{i \in M_2} S_i = K/2$ cannot hold.

If $\sum_{i \in M_1} S_i > K/2$ holds, then $\sum_{i \in M_1} S_i \geq K/2 + 1/2$ holds due to the integrality of S_i for $i \in I$. This together with (12), and

$$\phi \geq 1 - \varepsilon(K) = \left(\frac{K - \frac{1}{8K}}{K} \right)^2$$

leads to

$$\begin{aligned}
q_{(o,z_l^+)} &= \frac{K}{2} - \sqrt{\phi} \sum_{i \in M_1} S_i \\
&\leq \frac{K}{2} - \sqrt{\phi} \left(\frac{K}{2} + \frac{1}{2} \right) \\
&\leq \frac{K}{2} - \left(\frac{K - \frac{1}{8K}}{K} \right) \left(\frac{K}{2} + \frac{1}{2} \right) \\
&= \frac{K^2}{2K} - \frac{K^2 - \frac{1}{8}}{2K} - \frac{K - \frac{1}{8K}}{2K} = \frac{\frac{1}{8}}{2K} - \frac{K - \frac{1}{8K}}{2K} \\
&< 0,
\end{aligned}$$

which is a contradiction to $q_{(o,z_l^+)} \geq 0$. In analogy it follows that $\sum_{i \in M_2} S_i > K/2$ cannot hold.

Consequently, $\sum_{i \in M_1} S_i < K/2$ and $\sum_{i \in M_2} S_i < K/2$ hold. Due to the integrality of S_i for $i \in I$, $\sum_{i \in M_1} S_i \leq K/2 - 1/2$ and $\sum_{i \in M_2} S_i \leq K/2 - 1/2$ are satisfied. From this, (12), and $\phi < 1$, which holds due to Lemma 4.7, it follows

$$\begin{aligned}
q_{(o,z_l^+)} &= \frac{K}{2} - \sqrt{\phi} \sum_{i \in M_1} S_i \geq \frac{K}{2} - \sum_{i \in M_1} S_i \geq \frac{1}{2}, \\
q_{(z_l^+,w)} &= \frac{K}{2} - \sqrt{\phi} \sum_{i \in M_2} S_i \geq \frac{K}{2} - \sum_{i \in M_2} S_i \geq \frac{1}{2}.
\end{aligned}$$

This, Equalities (10), $\phi < 1$, and $S_l \leq K$ lead to

$$\begin{aligned}\left(q_{(o,z_l^+)} + q_{(z_l^+,w)}\right)^2 &= q^2_{(o,z_l^+)} + q^2_{(z_l^+,w)} + 2q_{(o,z_l^+)}q_{(z_l^+,w)} \\ &\geq \phi S_l^2 + 2 \cdot \frac{1}{4} \\ &> \phi S_l^2 + 2\frac{1}{8K}\sqrt{\phi}S_l + \left(\frac{1}{8K}\right)^2 \\ &= \left(\sqrt{\phi}S_l + \frac{1}{8K}\right)^2,\end{aligned}$$

and consequently, we obtain

$$q_{(o,z_l^+)} + q_{(z_l^+,w)} > \sqrt{\phi}S_l + \frac{1}{8K}. \tag{13}$$

From (9), (11), (13), and $\sum_{i\in I} S_i = K$ we obtain

$$\begin{aligned}K &= \sum_{i\in M_1} q_{(o,z_i^+)} + \sum_{i\in M_2} q_{(z_i^+,w)} + q_{(o,z_l^+)} + q_{(z_l^+,w)} \\ &= \sqrt{\phi}\sum_{i\in I\setminus\{l\}} S_i + q_{(o,z_l^+)} + q_{(z_l^+,w)} \\ &= \sqrt{\phi}(K - S_l) + q_{(o,z_l^+)} + q_{(z_l^+,w)} \\ &> \sqrt{\phi}(K - S_l) + \sqrt{\phi}S_l + \frac{1}{8K} \\ &= \sqrt{\phi}K + \frac{1}{8K},\end{aligned}$$

and consequently,

$$\frac{K - \frac{1}{8K}}{K} > \sqrt{\phi}$$

holds. This is a contradiction to the assumption

$$\phi \geq 1 - \varepsilon(K) = \left(\frac{K - \frac{1}{8K}}{K}\right)^2. \qquad \square$$

We have proven that the optimal value of (5) does not exceed the threshold $1-\varepsilon(K)$ if exactly one index $i \in I$ with $q_{(o,z_i^+)} > 0$ and $q_{(z_i^+,w)} > 0$ exists and Partition is infeasible. We now use this result to show that if arbitrarily many indices satisfy the latter property, the optimal objective value of (5) is bounded above by a threshold value smaller than 1. To this end, we consider two cases. In Lemma 4.11 at most one index $i \in I$ satisfies the more strict property $q_{(o,z_i^+)} \geq \varepsilon(K) > 0$ and $q_{(z_i^+,w)} \geq \varepsilon(K) > 0$ where $\varepsilon(K)$, defined in (3a), is a positive lower arc flow bound. Afterward, we consider that at least two indices satisfy this lower arc flow bound; see Lemma 4.12. To this end, we first prove two technical propositions that we use in the following.

In the next proposition, we show that a feasible point for (1a), (5b), and (5c) with a minimum potential difference between o and w can be modified to a feasible point of (5) while preserving the potential difference between o and w.

Proposition 4.9. Let $M \geq 0$ and (ℓ, q) be a feasible point for (1a), (5b), (5c), and for all $i \in I$

$$\Lambda_{(o,z_i^+)}q^2_{(o,z_i^+)} + \Lambda_{(z_i^+,w)}q^2_{(z_i^+,w)} \geq M$$

holds. Then, a point $(\tilde{\ell}, \tilde{q}, \pi)$ satisfying (1a), (5b), (5c), and additionally (1b) with

$$\Lambda_{(o,z_i^+)} \tilde{q}^2_{(o,z_i^+)} + \Lambda_{(z_i^+,w)} \tilde{q}^2_{(z_i^+,w)} = M$$

for all $i \in I$ exists. Moreover, $(\tilde{\ell}, \tilde{q}, \pi)$ is a feasible point for (5) with objective value of M.

Proof. Let (ℓ, q) be a point that satisfies the requirements. Since (ℓ, q) satisfies (1a) and (5c) for graph $G(\mathsf{Part})$, the flow q cannot contain any cycle flow. Thus, we obtain a flow decomposition as in Lemma 3.1 by applying Theorem 3.5 of [1]. Due to $q_a \geq 0$ for $a \in A$ and the graph structure of $G(\mathsf{Part})$, this flow decomposition satisfies that a positive flow $q_{(o,z_i^+)} > 0$, respectively $q_{(z_i^+,w)} > 0$ for any $i \in I$ can only be the result of a positive flow $q(P(u,v))$ with $P(u,v)$ being one of the following flow-paths

$$P(o, z_i^-) = (\{o, z_i^+, z_i^-\}, \{(o, z_i^+), (z_i^+, z_i^-)\}), \tag{14a}$$

$$P(z_i^+, w) = (\{z_i^+, w\}, \{(z_i^+, w)\}), \tag{14b}$$

$$P_i(o, w) = (\{o, z_i^+, w\}, \{(o, z_i^+), (z_i^+, w)\}). \tag{14c}$$

For every $i \in I$ with

$$\Lambda_{(o,z_i^+)} q^2_{(o,z_i^+)} + \Lambda_{(z_i^+,w)} q^2_{(z_i^+,w)} > M$$

we decrease positive flows $q(P(u,v))$ with $P(u,v)$ of (14) until

$$\Lambda_{(o,z_i^+)} q^2_{(o,z_i^+)} + \Lambda_{(z_i^+,w)} q^2_{(z_i^+,w)} = M \tag{15}$$

holds. This is possible due to Lemma 3.4. Furthermore, (1a), (5b), (5c) are still satisfied.

Due to (15) and (5c), we now can define the following potentials

$$\pi_o = \pi_o^+, \quad \pi_{z_i^+} = \pi_o - \Lambda_{(o,z_i^+)} q^2_{(o,z_i^+)}, \ i \in I, \tag{16a}$$

$$\pi_{z_i^-} = \pi_{z_i^+} - \Lambda_{(z_i^+,z_i^-)} q^2_{(z_i^+,z_i^-)}, \quad \pi_w = \pi_{z_i^+} - \Lambda_{(z_i^+,w)} q^2_{(z_i^+,w)}, \quad i \in I, \tag{16b}$$

which satisfy (1b) and $\pi_o - \pi_w = M$. □

In the next proposition, we prove that for every optimal solution of (5) an optimal solution with a specific flow decomposition exists. Moreover, the flows on arcs of the flow-paths $P_i(o, w)$ for all $i \in I$ do not differ between the two considered optimal solutions.

Proposition 4.10. Let $\mathsf{Partition}$ be infeasible. Let (ℓ, q, π) be an optimal solution of (5). Then an optimal solution $(\tilde{\ell}, \tilde{q}, \tilde{\pi})$ of (5) with a flow decomposition of Lemma 3.1 exists such that if $q(P(u,v)) > 0$, then $P(u,v)$ is defined by either (14a) or (14b). Additionally, $q_{(o,z_i^+)} = \tilde{q}_{(o,z_i^+)}$ and $q_{(z_i^+,w)} = \tilde{q}_{(z_i^+,w)}$ for $i \in I$ is satisfied.

Proof. Let (ℓ, q, π) be an optimal solution of (5) with objective value ϕ. From Lemma 4.7, it follows $\phi < 1$. Due to this, (1b), and (5c), flows q satisfy $q_{(o,z_i^+)} < S_i$ and $q_{(z_i^+,w)} < S_i$ for $i \in I$. We now consider a flow decomposition of Lemma 3.1 corresponding to solution (ℓ, q, π). Since $q_a \geq 0$ for $a \in A$ holds and the graph structure of $G(\mathsf{Part})$, this flow decomposition can be chosen such that $q(P(u,v))$ can only be positive for a flow-path $P(u,v)$ of (14) or $P(z_i^+, z_i^-)$ consisting of arc (z_i^+, z_i^-) for an $i \in I$, which follows from Theorem 3.5 in [1].

If $q(P(z_i^+, z_i^-)) > 0$ for an index $i \in I$ holds, then we delete this flow. We note that this does not modify flow on arcs (o, z_i^+), respectively (z_i^+, w), for $i \in I$. Thus, the modified nomination and flows $(\tilde{\ell}, \tilde{q})$ can be extended to a solution $(\tilde{\ell}, \tilde{q}, \tilde{\pi})$ of (5) with objective value ϕ, where the potentials $\tilde{\pi}$ are given by (16). Consequently, we can assume w.l.o.g. $q(P(z_i^+, z_i^-)) = 0$ for $i \in I$ in the remaining proof.

We now consider $i \in I$ with $q(P_i(o, w)) = \varepsilon > 0$. Due to $q_{(o,z_i^+)} < S_i$ and $q_{(z_i^+,w)} < S_i$ for $i \in I$, booking b, and (5c), we can set $q(P_i(o, w)) = \varepsilon > 0$ to zero and increase $q(P(o, z_i^-))$ and $q(P(z_i^+, w))$ by ε such that the corresponding solution $(\tilde{\ell}, \tilde{q})$ satisfies (5b), (5c), and (1a). We note that

$$\tilde{\ell}_{z_i^-} = \ell_{z_i^-} + \varepsilon \leq b_{z_i^-} = S_i$$

holds since before the modification $q(P(o, z_i^-)) = \ell_{z_i^-}$ and, thus,

$$q_{(o,z_i^+)} = q(P_i(o, w)) + q(P(o, z_i^-)) = \varepsilon + \ell_{z_i^-} < S_i$$

were satisfied. In analogy it follows $\tilde{\ell}_{z_i^+} = \ell_{z_i^+} + \varepsilon \leq b_{z_i^+} = S_i$. Additionally, we note that the flow on arc (o, z_i^+), respectively (z_i^+, w), for $i \in I$ is not modified. We now repeat the above procedure for every $i \in I$ with $q(P_i(o, w)) = \varepsilon > 0$. Afterward, we can extend the modified nomination and flows $(\tilde{\ell}, \tilde{q})$ to a solution $(\tilde{\ell}, \tilde{q}, \tilde{\pi})$ of (5) with objective value ϕ, where the potentials $\tilde{\pi}$ are given by (16). Due to the modification, $q_{(o,z_i^+)} = \tilde{q}_{(o,z_i^+)}$ and $q_{(z_i^+,w)} = \tilde{q}_{(z_i^+,w)}$ for $i \in I$ hold and the required flow decomposition is constructed. □

For the case that Partition is infeasible, we now prove that if in an optimal solution of (5) for at most one $i \in I$ the flow on the arcs (o, z_i^+) and (z_i^+, w) exceeds $\varepsilon(K)$, then the corresponding objective value is below the threshold $1 - \varepsilon(K) + \varepsilon(K)^2$.

Lemma 4.11. Let Partition be infeasible. Let

$$\varepsilon(K) = 1 - \left(\frac{K - \frac{1}{8K}}{K}\right)^2 \in (0, 1)$$

and (ℓ, q, π) be an optimal solution of (5) that satisfies

$$\left|\left\{i \in I : q_{(o,z_i^+)} \geq \varepsilon(K), q_{(z_i^+,w)} \geq \varepsilon(K)\right\}\right| \leq 1. \tag{17}$$

Then, the objective value ϕ corresponding to solution (ℓ, q, π) satisfies

$$\phi < 1 - \varepsilon(K) + \varepsilon(K)^2 < 1.$$

Proof. We contrarily assume that (ℓ, q, π) is an optimal solution of (5) that satisfies the requirements and its objective value is $\phi \geq 1 - \varepsilon(K) + \varepsilon(K)^2$. We further assume w.l.o.g. that the corresponding flow decomposition of Lemma 3.1 satisfies Proposition 4.10. From Lemma 4.7, it follows that $\phi < 1$. In the following, we consider the flow-paths (14) and partition the index set I as in (8).

Due to $\phi \geq 1 - \varepsilon(K) + \varepsilon(K)^2$ and Lemmas 4.6 and 4.8, $|M_3| \geq 2$ holds. For all $i \in I$, the inequality

$$q_{(o,z_i^+)}^2 + q_{(z_i^+,w)}^2 = \phi S_i^2, \tag{18}$$

follows from (1b) and (5c). Thus, the inequality $q_{(o,z_i^+)} > \varepsilon(K)$ or $q_{(z_i^+,w)} > \varepsilon(K)$ holds due to

$$q_{(o,z_i^+)}^2 + q_{(z_i^+,w)}^2 = \phi S_i^2 \ \geq \phi \geq 1 - \varepsilon(K) + \varepsilon(K)^2 > 2\varepsilon(K)^2,$$

where the latter inequality is valid due to

$$0 < \varepsilon(K) = 1 - \left(\frac{K - \frac{1}{8K}}{K}\right)^2 = 1 - (1 - \frac{1}{8K^2})^2 \leq 1 - \frac{49}{64} = \frac{15}{64}.$$

We now set $q_a = 0$ for each $a = (u, v) \in \{(o, z_i^+) : i \in I\} \cup \{(z_i^+, w) : i \in I\}$ that satisfies $q_a \leq \varepsilon(K)$. This can be done in the considered flow decomposition by decreasing flows $q(P(o, z_i^-))$, respectively $q(P(z_i^+, w))$ for $i \in I$. We denote the modified flows by $\tilde{q}$ and its corresponding nomination by $\tilde{\ell}$, which satisfy (1a), (5b), and (5c). We further note that now $|M_3| \leq 1$ holds, due to (17).

For an arbitrary index $i \in I$, we assume that $q_{(z_i^+, w)}$ has been modified, i.e., $\tilde{q}_{(z_i^+, w)} = 0 < q_{(z_i^+, w)}$. Consequently, $\tilde{q}_{(o, z_i^+)} = q_{(o, z_i^+)}$ holds. This together with (18), $\phi \geq 1 - \varepsilon(K) + \varepsilon(K)^2$, and $S_i \geq 1$ leads to

$$\begin{aligned} \tilde{q}^2_{(z_i^+, w)} + \tilde{q}^2_{(o, z_i^+)} &= \tilde{q}^2_{(o, z_i^+)} = q^2_{(o, z_i^+)} = \phi S_i^2 - q^2_{(z_i^+, w)} \\ &\geq \phi S_i^2 - \varepsilon(K)^2 \geq (1 - \varepsilon(K) + \varepsilon(K)^2) S_i^2 - \varepsilon(K)^2 \\ &\geq (1 - \varepsilon(K)) S_i^2. \end{aligned}$$

In analogy, we can handle the case that $q_{(o, z_i^+)}$ has been modified.

Due to this and $\Lambda_{(o, z_i^+)} = \Lambda_{(z_i^+, w)} = 1/S_i^2$, we can apply Proposition 4.9 and obtain a solution $(\tilde{\ell}, \tilde{q}, \tilde{\pi})$ for (5) with objective value $\tilde{\phi} \geq 1 - \varepsilon(K) > 0$. This solution satisfies $|M_3| \leq 1$ due to the modification, (17), and the fact that we only possibly decrease flows in Proposition 4.9 to obtain $(\tilde{\ell}, \tilde{q}, \tilde{\pi})$.

If $|M_3| = 1$ holds, then this is a direct contradiction to Lemma 4.8.

We now assume $|M_3| = 0$. Due to $|M_3| \geq 2$ before the modification and the requirements, at least one arc flow was decreased by the above. Consequently, $\tilde{\ell}_o < K/2$ or $\tilde{\ell}_w < K/2$ holds. Furthermore, $|M_1| \geq 1$ or $|M_2| \geq 1$ is satisfied after the modification. We now modify the solution such that its objective stays the same but $|M_3| = 1$ holds which is a contradiction to Lemma 4.8.

Let be $\tilde{\ell}_o < K/2$ and $\tilde{\ell}_w < K/2$. We assume w.l.o.g. that $q_{(o, z_i^+)} > 0$ holds for some $i \in I$. Due to the considered flow decomposition and Lemma 3.4, we now can decrease $q(P(o, z_i^-))$ by $\varepsilon > 0$ and increase $q(P(z_i^+, w))$ by $\tilde{\varepsilon} > 0$ such that both arc flows $\tilde{q}_{(o, z_i^+)}$ and $\tilde{q}_{(z_i^+, w)}$ are positive, the potential drop $\Pi_{P_i(o,w)}$ stays the same, and $\tilde{\ell} \leq b$ holds. Consequently, $|M_3| = 1$ is satisfied for the modified solution $(\tilde{\ell}, \tilde{q}, \tilde{\pi})$ and its objective value $\tilde{\phi}$ satisfies $\tilde{\phi} \geq 1 - \varepsilon(K)$, which is a contradiction to Lemma 4.8.

Let be $\tilde{\ell}_o < K/2$ and $\tilde{\ell}_w = K/2$. From this and (1a), it follows that $q_{(z_i^+, w)} > 0$ exists. Due to the considered flow decomposition and Lemma 3.4, we can decrease $q(P(z_i^+, w))$ by $\varepsilon > 0$ and increase $q(P_i(o, w))$ by $\tilde{\varepsilon}$ with $\varepsilon \geq \tilde{\varepsilon} > 0$ such that the potential drop $\Pi_{P_i(o,w)}$ stays the same, $\tilde{\ell} \leq b$, and $\tilde{q}_{(o, z_i^+)}$ and $\tilde{q}_{(z_i^-, w)}$ are positive. Consequently, $|M_3| = 1$ is satisfied for the modified solution $(\tilde{\ell}, \tilde{q}, \tilde{\pi})$ and its objective value $\tilde{\phi}$ satisfies $\tilde{\phi} \geq 1 - \varepsilon(K)$, which is a contradiction to Lemma 4.8. In analogy, we handle the case $\tilde{\ell}_o = K/2$ and $\tilde{\ell}_w < K/2$. □

We now consider the counterpart of Lemma 4.11, i.e.,

$$\left|\left\{i \in I : q_{(o, z_i^+)} \geq \varepsilon(K), q_{(z_i^+, w)} \geq \varepsilon(K)\right\}\right| \geq 2. \tag{19}$$

Lemma 4.12. Let Partition be infeasible. Let

$$\varepsilon(K) = 1 - \left(\frac{K - \frac{1}{8K}}{K}\right)^2 \in (0, 1)$$

and (ℓ, q, π) be a solution of (5) that satisfies (19). Then, the corresponding objective value ϕ satisfies

$$\phi < 1 - \frac{\varepsilon(K)^2}{K^2} < 1.$$

Proof. We contrarily assume that a solution (ℓ, q, π) of (5) satisfying (19) with an objective value $\phi \geq 1 - \varepsilon(K)^2/K^2$ exists. From Lemma 4.7, it follows $\phi < 1$. Due to (19), $l \neq r \in I$ with

$$q_{(o,z_l^+)} \geq \varepsilon(K), \; q_{(z_l^+,w)} \geq \varepsilon(K), \quad q_{(o,z_r^+)} \geq \varepsilon(K), \; q_{(z_r^+,w)} \geq \varepsilon(K)$$

exist. This and

$$q^2_{(o,z_l^+)} + q^2_{(z_l^+,w)} = \phi S_l^2, \quad q^2_{(o,z_r^+)} + q^2_{(z_r^+,w)} = \phi S_r^2,$$

lead, in analogy to (13), to the inequalities

$$q_{(o,z_l^+)} + q_{(z_l^+,w)} > \sqrt{\phi} S_l + \frac{\varepsilon(K)^2}{2K}, \quad q_{(o,z_r^+)} + q_{(z_r^+,w)} > \sqrt{\phi} S_r + \frac{\varepsilon(K)^2}{2K}. \tag{20}$$

We now consider the partition M_1, M_2, and M_3 of I according to (8). Consequently, (11) is satisfied. From this, flow conservation (1a), and booking b, it follows

$$\begin{aligned}
\frac{K}{2} &\geq \sum_{i \in M_1 \cup M_3} q_{(o,z_i^+)} \geq \sqrt{\phi} \sum_{i \in M_1} S_i + \sum_{i \in M_3} q_{(o,z_i^+)}, \\
\frac{K}{2} &\geq \sum_{i \in M_2 \cup M_3} q_{(z_i^+,w)} \geq \sqrt{\phi} \sum_{i \in M_2} S_i + \sum_{i \in M_3} q_{(z_i^+,w)}.
\end{aligned}$$

Combining the previous inequalities, $\sum_{i \in I} S_i = K$, Observation 4.4, (20), and $\phi \geq 1 - \varepsilon(K)^2/K^2$ lead to

$$\begin{aligned}
K &\geq \sqrt{\phi} \sum_{i \in M_1 \cup M_2} S_i + \sum_{i \in M_3} \left(q_{(o,z_i^+)} + q_{(z_i^+,w)} \right) \\
&\geq \sqrt{\phi} \sum_{i \in I \setminus \{l,r\}} S_i + q_{(o,z_l^+)} + q_{(z_l^+,w)} + q_{(o,z_r^+)} + q_{(z_r^+,w)} \\
&= \sqrt{\phi}(K - S_r - S_l) + q_{(o,z_l^+)} + q_{(z_l^+,w)} + q_{(o,z_r^+)} + q_{(z_r^+,w)} \\
&> \sqrt{\phi}(K - S_r - S_l) + \sqrt{\phi} S_l + \frac{\varepsilon(K)^2}{2K} + \sqrt{\phi} S_r + \frac{\varepsilon(K)^2}{2K} \\
&= \sqrt{\phi} K + \frac{\varepsilon(K)^2}{K}.
\end{aligned}$$

This leads to the contradiction

$$\frac{K - \frac{\varepsilon(K)^2}{K}}{K} = 1 - \frac{\varepsilon(K)^2}{K^2} > \sqrt{\phi} \geq \phi$$

because $1 > \phi \geq 1 - \varepsilon(K)^2/K^2 > 0$ holds. □

Lemmas 4.11 and 4.12 prove that if Partition is infeasible, then $\varphi^+_{ow}(b)$ can be bounded above by $M(K)$ given as

$$M(K) = \max \left\{ 1 - \varepsilon(K) + \varepsilon(K)^2, 1 - \frac{\varepsilon(K)^2}{K^2} \right\}, \quad \varepsilon(K) = 1 - \left(\frac{K - \frac{1}{8K}}{K} \right)^2,$$

where the coding length of $M(K)$ is polynomially bounded above by the coding length of the given Partition instance. In the following two lemmas, we prove an analogue statement for the case that the flow is not necessarily nonnegative, i.e., we consider the general maximum potential-difference problem (2) w.r.t. (o, w). To this end, $M(K)$ and $\tilde{\varepsilon}(K) = (1 - M(K))/5$ come into play; see (3). Moreover, we need the following auxiliary proposition.

Proposition 4.13. Let Partition be infeasible. Let (ℓ, q, π) be an optimal solution of (2) w.r.t. (o, w) with objective value $\phi > 0$. Further, there is at least one arc $a \in A$ with negative arc flow $q_a < 0$. Then, for all $i \in I$, the inequalities

$$\left|q_{(o,z_i^+)}\right| \leq S_i, \quad \left|q_{(z_i^+,w)}\right| \leq S_i, \tag{21}$$

hold.

Proof. Let (ℓ, q, π) be an optimal solution of (2) w.r.t. (o, w) that satisfies the requirements. For all $i \in I$, the inequality $q_{(z_i^+,z_i^-)} \geq 0$ holds due to the structure of graph $G(\mathsf{Part})$. Moreover, for all $i \in I$, at least one of the arc flows $q_{(o,z_i^+)}$ and $q_{(z_i^+,w)}$ is positive due to $\phi > 0$. For every $i \in I$ for which either $q_{(o,z_i^+)} < 0$ or $q_{(z_i^+,w)} < 0$ hold, the flow bounds (21) follow from the graph structure of $G(\mathsf{Part})$, (1a), and the considered booking b. Further, there is at least one index $i \in I$ that satisfies (21) and either $q_{(o,z_i^+)} < 0$ or $q_{(z_i^+,w)} < 0$ due to the requirements. Consequently, $\phi < 1$ follows from

$$\phi = \pi_o - \pi_w = \frac{1}{S_i^2} q_{(o,z_i^+)} \left|q_{(o,z_i^+)}\right| + \frac{1}{S_i^2} q_{(z_i^+,w)} \left|q_{(z_i^+,w)}\right| < 1. \tag{22}$$

Moreover, from Relation (22), it follows that for $i \in I$ with $q_{(o,z_i^+)} \geq 0$ and $q_{(z_i^+,w)} \geq 0$ Inequalities (21) are satisfied. $\square$

Lemma 4.14. Let Partition be infeasible and $n \geq 3$ denotes the number of elements of the considered partition instance. Let $M(K)$ and $\tilde{\varepsilon}(K)$ be given as in (3) and (ℓ, q, π) be an optimal solution of (2) w.r.t. (o, w) with objective value ϕ. If this solution satisfies $|q_a| \leq \tilde{\varepsilon}(K)/n$ for each $a \in A$ with $q_a < 0$, then

$$\phi < M(K) + 4\tilde{\varepsilon}(K) < 1$$

holds.

Proof. We contrarily assume that an optimal solution (ℓ, q, π) for (2) w.r.t. (o, w) with objective value ϕ that satisfies the requirements, explicitly $|q_a| \leq \tilde{\varepsilon}(K)/n$ for $a \in A$ with $q_a < 0$, exists and $\phi \geq M(K) + 4\tilde{\varepsilon}(K)$ holds.

If $q_a \geq 0$ holds for all $a \in A$, then this is a contradiction to Lemma 4.11 or 4.12 due to the objective value $\phi \geq M(K) + 4\tilde{\varepsilon}(K)$.

Now at least one arc $a \in A$ satisfies $q_a < 0$. From the graph structure of $G(\mathsf{Part})$ and booking b, it follows $q_{(z_i^+,z_i^-)} \geq 0$ for all $i \in I$. Since $\phi > 0$ and (1b), for every $i \in I$ at least one arc flow $q_{(o,z_i^+)}$ or $q_{(z_i^+,w)}$ is positive. Consequently, at most n arcs with negative flow exist. Moreover, from Proposition 4.13, it follows that the flow bounds (21) are satisfied for $i \in I$. Additionally, $q_{(o,z_i^+)} > \tilde{\varepsilon}(K)$ or $q_{(z_i^+,w)} > \tilde{\varepsilon}(K)$ holds for every $i \in I$ because of

$$q_{(o,z_i^+)} \left|q_{(o,z_i^+)}\right| + q_{(z_i^+,w)} \left|q_{(z_i^+,w)}\right| = \phi S_i^2 \geq \phi \geq M(K) + 4\tilde{\varepsilon}(K) > 2\tilde{\varepsilon}(K)^2.$$

We now consider a flow decomposition of Lemma 3.1. For every arc $a \in A$ with $q_a < 0$, we delete every positive flow $q(P(u, v))$ where the flowpath $P(u, v)$ satisfies $\chi_a(P) = -1$. Consequently, we obtain $\tilde{q}_a \geq 0$ for $a \in A$ with corresponding nomination $\tilde{\ell}$. Due to the chosen flow decomposition and maximally n arcs a

with negative arc flow, satisfying $|q_a| \leq \tilde{\varepsilon}(K)/n$, exist, this modification maximally decreases an arbitrary arc flow by $n(\tilde{\varepsilon}(K)/n) = \tilde{\varepsilon}(K)$. Further, the flow bounds (21) still hold for $i \in I$. If either $q_{(o,z_i^+)} > \tilde{\varepsilon}(K)$ or $q_{(z_i^+,w)} > \tilde{\varepsilon}(K)$ holds, then we assume w.l.o.g. that $q_{(o,z_i^+)} > \tilde{\varepsilon}(K)$ is satisfied. This leads to

$$\begin{aligned}
\tilde{q}^2_{(o,z_i^+)} + \tilde{q}^2_{(z_i^+,w)} &\geq \left(\max\left\{0, q_{(o,z_i^+)} - \tilde{\varepsilon}(K)\right\}\right)^2 + \left(\max\left\{0, q_{(z_i^+,w)} - \tilde{\varepsilon}(K)\right\}\right)^2 \\
&= q^2_{(o,z_i^+)} - 2q_{(o,z_i^+)}\tilde{\varepsilon}(K) + \tilde{\varepsilon}(K)^2 \\
&\geq q^2_{(o,z_i^+)} - 2q_{(o,z_i^+)}\tilde{\varepsilon}(K) + q^2_{(z_i^+,w)} \\
&\geq \phi S_i^2 - 2q_{(o,z_i^+)}\tilde{\varepsilon}(K) \\
&\geq \phi S_i^2 - 2S_i\tilde{\varepsilon}(K) \ \geq (M(K) + 4\tilde{\varepsilon}(K))S_i^2 - 2S_i\tilde{\varepsilon}(K) \\
&\geq M(K)S_i^2.
\end{aligned}$$

If $q_{(o,z_i^+)} > \tilde{\varepsilon}(K)$ and $q_{(z_i^+,w)} > \tilde{\varepsilon}(K)$ hold, then this leads to

$$\begin{aligned}
\tilde{q}^2_{(o,z_i^+)} + \tilde{q}^2_{(z_i^+,w)} &\geq \left(\max\left\{0, q_{(o,z_i^+)} - \tilde{\varepsilon}(K)\right\}\right)^2 + \left(\max\left\{0, q_{(z_i^+,w)} - \tilde{\varepsilon}(K)\right\}\right)^2 \\
&= q^2_{(o,z_i^+)} - 2q_{(o,z_i^+)}\tilde{\varepsilon}(K) + \tilde{\varepsilon}(K)^2 + q^2_{(z_i^+,w)} - 2q_{(z_i^+,w)}\tilde{\varepsilon}(K) + \tilde{\varepsilon}(K)^2 \\
&\geq \phi S_i^2 - 2q_{(o,z_i^+)}\tilde{\varepsilon}(K) - 2q_{(z_i^+,w)}\tilde{\varepsilon}(K) \\
&\geq \phi S_i^2 - 4S_i\tilde{\varepsilon}(K) \ \geq (M(K) + 4\tilde{\varepsilon}(K))S_i^2 - 4S_i\tilde{\varepsilon}(K) \\
&\geq M(K)S_i^2.
\end{aligned}$$

Thus, the modification decreases the potential drop $\Pi_{P_i(o,w)}$, but it is at least $M(K)$. Furthermore, $\tilde{q} \geq 0$ holds and we only decreased flows of q to obtain $\tilde{q}$. Consequently, $(\tilde{\ell}, \tilde{q})$ satisfy (1a), (5b), and (5c). Due to this and $\Lambda_{(o,z_i^+)} = \Lambda_{(z_i^+,w)} = 1/S_i^2$, we can apply Proposition 4.9 and obtain a feasible point of (2) w.r.t. (o, w) with $q_a \geq 0$ and objective value of at least $M(K)$. But this is a contradiction to Lemma 4.11 or 4.12. □

We now prove that if Partition is infeasible and in an optimal solution of (2) w.r.t. (o, w) at least one negative arc flow has an absolute flow of at least $\tilde{\varepsilon}(K)/n$, then we can bound the objective of (2) as follows.

Lemma 4.15. Let Partition be infeasible. Further, let $\varepsilon(K)$, $M(K)$, and $\tilde{\varepsilon}(K)$ be given as in (3). Moreover, let (ℓ, q, π) be a feasible point of (2) w.r.t. (o, w) such that at least one arc $a \in A$ satisfies $q_a < 0$ and $|q_a| \geq \tilde{\varepsilon}(K)/n$. Then, the corresponding objective value ϕ satisfies

$$\phi < 1 - \frac{\tilde{\varepsilon}(K)^2}{K^2 n^2}.$$

Proof. We contrarily assume that a solution (ℓ, q, π) of (2) w.r.t. (o, w) with objective value

$$\phi \geq 1 - \frac{\tilde{\varepsilon}(K)^2}{K^2 n^2}$$

satisfies the requirements. Consequently, an arc $a \in A$ with $q_a < 0$ and $|q_a| \geq \tilde{\varepsilon}(K)/n$ exists. We now consider the case that $a = (o, z_i^+)$ for some $i \in I$ holds. Due to Proposition 4.13 and the value of $\phi \ > 0$, the flow bounds $0 \leq q_{(z_i^+,w)} \leq S_i$ are satisfied. This,

$$-q^2_{(o,z_i^+)} + q^2_{(z_i^+,w)} = \phi S_i^2 \geq \left(1 - \frac{\tilde{\varepsilon}(K)^2}{K^2 n^2}\right) S_i^2,$$

and $S_i < K$, lead to the contradiction

$$\begin{aligned}
1 - \frac{\tilde{\varepsilon}(K)^2}{K^2 n^2} &\leq \frac{q^2_{(z_i^+,w)} - q^2_{(o,z_i^+)}}{S_i^2} \\
&\leq 1 - \frac{q^2_{(o,z_i^+)}}{S_i^2} \leq 1 - \frac{\left(\frac{\tilde{\varepsilon}(K)}{n}\right)^2}{S_i^2} \\
&< 1 - \frac{\left(\frac{\tilde{\varepsilon}(K)}{n}\right)^2}{K^2} = 1 - \frac{\tilde{\varepsilon}(K)^2}{K^2 n^2}.
\end{aligned}$$

In analogy to the above, it follows the case of $a = (z_i^+, w)$ for some $i \in I$. □

Combining now the results of Lemmas 4.11–4.15, we can bound the objective of (2) w.r.t. (o, w) by the polynomial $T(K)$ given by (3b).

Lemma 4.16. Let Partition be infeasible. Let $M(K)$ and $\tilde{\varepsilon}(K)$ be given as in (3). Then,

$$\varphi_{ow}(b) < \max\left\{1 - \frac{\tilde{\varepsilon}(K)^2}{K^2 n^2}, M(K) + 4\tilde{\varepsilon}(K)\right\} = T(K) < 1$$

holds.

Proof. Let (ℓ, q, π) be an optimal solution of (2) w.r.t. (o, w). If $q_a \geq 0$ for $a \in A$ holds, then the claim follows from Lemmas 4.11 and 4.12. If an arc $a \in A$ with $q_a < 0$ exists, then the claim follows from Lemmas 4.14 and 4.15. □

Since the feasibility of a booking can be characterized by the nominations with maximum potential-difference, see (4), the previous lemma connects the feasibility of Partition to (2) w.r.t. (o, w).

Lemma 4.17. Partition is feasible if and only if $\varphi_{ow}(b) > T(K)$ is satisfied.

Proof. If Partition is infeasible, then from Lemma 4.16 it follows $\varphi_{ow}(b) < T(K) < 1$. If Partition is feasible, then from Lemma 4.3 it follows $\varphi_{ow}(b) \geq 1 > T(K)$, since $T(K) < 1$. □

With the help of the previous result and using again the characterization of a feasible booking by (4), we connect the infeasibility of a booking and Partition.

Theorem 4.18. The booking b is infeasible if and only if Partition is feasible.

Proof. The claim follows from Corollary 4.2 and Lemma 4.17. □

Finally, we prove our main result that deciding the feasibility of a booking (FB) is coNP-hard.

Theorem 4.19. Deciding the feasibility of a booking (FB) is coNP-hard.

Proof. Deciding the feasibility of a booking is coNP-hard due to Theorem 4.18. □

We further note that deciding wether there exists a nomination with maximum potential-difference (MPD), see (2), of at least $T(K)$ is NP-hard.

Lemma 4.20. Computing a maximum potential-difference nomination (MPD) is NP-hard.

Proof. The claim follows from $T(K) < 1$ and Lemmas 4.17 and 4.3. □

MPD is still NP-hard with the additional restriction of nonnegative flow; see (5).

Lemma 4.21. Computing a maximum potential-difference nomination (MPD) with the additional restriction of nonnegative flow (5c) is NP-hard.

Proof. The claim follows from Lemma 4.3, its proof, Lemmas 4.11 and 4.12, and $T(K) < 1$. □

We close this section with a brief remark why the reduction of this section is not applicable to linear potential-based flows, i.e., considering q_a instead of $q_a|q_a|$ in (1b). For the latter, we know that FB is in P; see [25].

The hardness proof of FB w.r.t. nonlinear potential-based flow model (1) is based on Observation 4.4. It implies that if $q_{(o,z_i^+)} > 0$ and $q_{(z_i^+,w)} > 0$ hold, then we need strictly more flow in terms of $q_{(o,z_i^+)} + q_{(z_i^+,w)}$ to obtain a pressure drop of ϕ, i.e., $\Lambda_{(o,z_i^+)} q^2_{(o,z_i^+)} + \Lambda_{(z_i^+,w)} q^2_{(z_i^+,w)} = \phi$, in contrast to the case if one of the latter flows is zero. This does not apply if we consider a less accurate linear potential-based flow model. Thus, the previous reduction from Partition to the infeasibility of a booking is not applicable for a linear potential-based flow model.

5. Conclusion

In this paper, we prove that deciding the feasibility of a booking (FB) in the European entry-exit gas market considering a nonlinear potential-based flow model is coNP-hard in cyclic graphs. To this end, we reduced Partition to the infeasibility of a booking. This is the first hardness result for FB w.r.t. potential-based flows, since the latter is in P for linear potential-based flows in general graphs; see [25]. It is also in P for trees and a single-cycle network considering a nonlinear potential-based flow model; see [25, 26, 35]. Thus, it is finally shown that FB is hard and a first border separating the easy from the hard variants of the problem is given. Hence, main parts of the complexity regarding the considered problem are now understood; see Figure 1 for an overview. Moreover, we prove that computing a nomination with the maximum potential-difference is NP-hard even if we can determine the flow direction a priori. However, an open question is if we can sharpen the line that separates the easy from the hard cases of FB. A reasonable next case could be the class of cactus graphs since for trees and a single cycle the considered problem is in P and for cyclic graphs it is coNP-hard. Furthermore, it remains open if FB is strongly coNP-hard.

Our complexity analysis shows that FB is indeed a challenging problem for the transmission system operator (TSO) in the European entry-exit gas market system. Moreover, FB has to be solved by the TSO whenever a booking contract is signed. Thus, the development of effective models for FB, possibly using the structural knowledge of our complexity analysis, offers new possibilities for future research.

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Article 5

A Bilevel Optimization Approach to Decide the Feasibility of Bookings in the European Gas Market

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ORIGINAL ARTICLE

A bilevel optimization approach to decide the feasibility of bookings in the European gas market

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Abstract

The European gas market is organized as a so-called entry-exit system with the main goal to decouple transport and trading. To this end, gas traders and the transmission system operator (TSO) sign so-called booking contracts that grant capacity rights to traders to inject or withdraw gas at certain nodes up to this capacity. On a day-ahead basis, traders then nominate the actual amount of gas within the previously booked capacities. By signing a booking contract, the TSO guarantees that all nominations within the booking bounds can be transported through the network. This results in a highly challenging mathematical problem. Using potential-based flows to model stationary gas physics, feasible bookings on passive networks, i.e., networks without controllable elements, have been characterized in the recent literature. In this paper, we consider networks with linearly modeled active elements such as compressors or control valves. Since these active elements allow the TSO to control the gas flow, the single-level approaches for passive networks from the literature are no longer

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applicable. We thus present a bilevel model to decide the feasibility of bookings in networks with active elements. While this model is well-defined for general active networks, we focus on the class of networks for which active elements do not lie on cycles. This assumption allows us to reformulate the original bilevel model such that the lower-level problem is linear for every given upper-level decision. Consequently, we derive several single-level reformulations for this case. Besides the classic Karush–Kuhn–Tucker reformulation, we obtain three problem-specific optimal-value-function reformulations. The latter also lead to novel characterizations of feasible bookings in networks with active elements that do not lie on cycles. We compare the performance of our methods by a case study based on data from the GasLib.

Keywords Gas networks · Bilevel optimization · European entry-exit market · Bookings · Active elements

Mathematics Subject Classification 90B10 · 90C11 · 90C35 · 90C46 · 90C90

1 Introduction

The main goal of the European entry-exit gas market is to decouple transport and trading of gas. The transmission system operator (TSO), who operates the network, and gas traders interact via so-called bookings. A booking represents a mid- to long-term capacity-right contract between gas traders and the TSO. It grants traders the right to inject and withdraw gas up to the booked capacities at certain nodes of the network. After signing these booking contracts, gas traders can nominate on a daily basis the actual quantities of gas within their booked capacities that should be shipped through the network by the TSO. In total, these so-called nominations have to be balanced and represent the quantities of gas that are injected at entry nodes or withdrawn at exit nodes in a single time period.

By signing a booking contract, the TSO is obliged to guarantee that every balanced and booking-compliant load flow can be transported through the network, which follows from the European directive (Directive 2009) and the subsequent regulation (European Parliament Council 2009) on the entry-exit gas market. Indeed, this condition decouples transport and trading, since after signing the booking contracts, the gas traders can nominate any balanced quantity of gas without considering any transport requirements of the network. However, from a mathematical point of view, deciding the feasibility of a booking poses a significant challenge since infinitely many different balanced load flows have to be checked for being transportable through the network.

First mathematical results regarding bookings are obtained in the PhD theses by Hayn (2016) and Willert (2014). Some structural properties of bookings are analyzed in Willert (2014). Further, Hayn (2016) studies the problem of deciding the feasibility of a booking as a quantifier elimination problem and presents an algorithm that decides the feasibility of a booking in an active network up to a certain tolerance. The remaining literature regarding bookings focuses on the case of passive networks. In Fügenschuh et al. (2014), the so-called reservation-allocation problem is studied for linear flow problems, which is closely related to the feasibility of a booking. Later on, in Labbé et al. (2020), a characterization of feasible bookings is obtained, in which for each pair of nodes, a nonlinear optimization problem needs to be solved to global optimality. These nonlinear problems compute the maximum pressure difference between the corresponding two nodes that can be obtained within the considered booking. If these maximum pressure differences satisfy certain pressure bounds, the booking is feasible and otherwise, it is infeasible. This characterization can be used to decide the feasibility of a booking in polynomial time for passive, tree-shaped networks (Labbé et al. 2020) or passive, single-cycle networks (Labbé et al. 2021). However, the problem is coNP-hard on passive networks in general (Thürauf 2020). Moreover, optimizing over the set of feasible bookings is hard even on tree-shaped networks (Schewe et al. 2020). We note that deciding the feasibility of bookings can also be seen as a special two-stage robust or adjustable robust optimization problem in which the uncertainty set consists of balanced and booking-compliant load flows. Exploiting this point of view, the authors of Aßmann (2019); Aßmann et al. (2019); Robinius et al. (2019) derive methods that can be used to decide the feasibility of bookings in passive networks. Moreover, results of booking feasibility are not restricted to the European entry-exit gas market, but can also be applied to other potential-based network problems such as network expansion under demand uncertainties. This is demonstrated, e.g., in Robinius et al. (2019), where a robust diameter selection for hydrogen networks is computed that is protected against unknown future demand fluctuations.

Unfortunately, all these results in passive networks cannot be used directly to decide the feasibility of bookings in active networks. Switching from passive to active networks makes the problem even more challenging as it introduces binary decisions for switching on or off active elements such as compressors or control valves. These binary decisions have to be taken individually for each balanced load flow within the booking bounds, since the TSO is able to change the settings of the active elements. This additional degree of freedom leads us to consider the following bilevel structure. The upper-level adversarial player tries to find a balanced and booking-compliant load flow that cannot be transported. The TSO, acting as the lower-level player, uses the active elements to transport this "worst-case" load flow of the upper level through the network. Consequently, if the upper-level player finds a balanced and booking-compliant load flow that cannot be transported by the TSO in the lower level, then the booking is infeasible. Otherwise, it is feasible. For an introduction to bilevel optimization, we refer to the books Bard (1998); Dempe (2002) and the recent survey article see above Kleinert et al. (2021). In general, bilevel optimization has been successfully applied to many different problems in the context of energy networks; see Wogrin et al. (2020). Moreover, it has specifically been applied to find scenarios that lead to severe transport situations in passive gas networks with linear flow models; see, e.g., Hennig and Schwarz (2016).

In this paper, we present a first stepping stone towards deciding the feasibility of bookings in networks with linearly modeled active elements and a nonlinear model for stationary gas transport. First, a bilevel model for validating bookings on networks with active elements is derived. Since even linear bilevel optimization is computationally hard, see Hansen et al. (1992); Jeroslow (1985), and since we additionally consider nonlinear gas transport models, we assume that no active element is part of a cycle of the network; see, e.g., Aßmann et al. (2019), where this assumption is used as well. This allows us to reformulate our model as a bilevel problem with mixed-integer nonlinear upper level and a linear lower level. We then develop different approaches to solve this challenging bilevel problem. First, the classic Karush–Kuhn–Tucker (KKT) approach is applied. We provide provably correct bounds on the lower-level primal and dual variables to be used in the linearization of the KKT complementarity constraints. Then, three closed-form expressions of the lower-level optimal value function are studied. Using these closed-form formulas, we set up optimal-value-function reformulations of the presented bilevel model, which then lead to novel characterizations of feasible bookings in active networks. The obtained approaches are evaluated in a computational study for some instances of the GasLib (Schmidt et al. 2017). The results show that the nonlinear gas flow model is computationally very challenging, which only allows for a limited comparison of the methods. Thus, we also conducted a computational study for a simplified linear flow model.

The remainder of this paper is structured as follows. In Sect. 2, we formally introduce the problem of deciding the feasibility of a booking in networks with active elements. In Sect. 3, we then illustrate why the methods for the case of passive networks cannot be applied and how active elements make the problem even more challenging. We present a bilevel model for deciding the feasibility of a booking for active networks in Sect. 4. While this model is well-defined for general active networks, we afterward focus on networks in which the active elements do not lie on cycles. This assumption allows us to reformulate the original bilevel model such that the lower-level problem is linear for every given upper-level decision. Based on the reformulated bilevel model, we provide the single-level KKT reformulation in Sect. 5 and discuss various optimal-value-function reformulations and characterizations of feasible bookings in active networks in Sect. 6. We then compare our methods in a computational study in Sect. 7. Finally, we summarize our results and discuss possible directions for future research in Sect. 8.

2 Problem description

We now formalize the problem of deciding the feasibility of a booking in gas networks including compressors and control valves. We follow and extend the problem description in Labbé et al. (2021), which deals with the feasibility of a booking for a single-cycle network without active elements. To this end, we consider linearly modeled active elements and stationary gas flows.

We model a gas network by a weakly connected and directed graph $G = (V, A)$ with nodes V and arcs A. The set of nodes is partitioned into entry nodes V_+, at which gas is injected, exit nodes V_-, at which gas is withdrawn, and the remaining inner nodes V_0. The set of arcs is partitioned into pipes A_{pipe} and active elements A_{act}, which can actively control the pressure. Further, the set of active elements is split into compressors A_{cm}, which can increase the pressure, and control valves A_{cv}, which can decrease the pressure.

We now introduce our framework for deciding the feasibility of a booking.

Definition 2.1 A *load flow* is a vector $\ell = (\ell_u)_{u \in V} \in \mathbb{R}^V_{\geq 0}$ with $\ell_u = 0$ for all $u \in V_0$. The set of load flows is denoted by L.

A load flow leads to an actual flow situation in the gas network. More precisely, ℓ_u denotes the amount of gas that is injected at an entry $u \in V_+$ and that is withdrawn at an exit $u \in V_-$. Since we consider stationary gas flows, the quantities of gas injected and withdrawn from the network have to be balanced. This leads to the definition of a nomination.

Definition 2.2 A *nomination* is a balanced load flow ℓ, i.e., $\sum_{u \in V_+} \ell_u = \sum_{u \in V_-} \ell_u$. The set of nominations is given by

$$N := \left\{ \ell \in L : \sum_{u \in V_+} \ell_u = \sum_{u \in V_-} \ell_u \right\}.$$

A booking, on the other hand, represents a mid- to long-term contract in the European entry-exit gas market between the gas traders and the TSO that allows gas traders to inject or withdraw gas at certain nodes up to the booked capacity. To do so, the TSO is obliged to guarantee that all possibly infinitely many booking-compliant nominations can be transported through the network.

Definition 2.3 A *booking* is a load flow $b \in L$. A nomination ℓ is called *booking-compliant* w.r.t. the booking b if $\ell \leq b$ holds, where "$\leq$" is meant component-wise throughout this paper. The set of booking-compliant nominations is given by $N(b) := \{\ell \in N : \ell \leq b\}$.

In the following, we consider stationary gas flows based on the Weymouth pressure loss equation (Weymouth 1912). In line with the corresponding literature Schewe et al. (2020), Thürauf (2020), and Labbé et al. (2021), we model gas flow physics using potential-based flows, which for active networks consist of arc flows $q = (q_a)_{a \in A}$, node potentials $\pi = (\pi_u)_{u \in V}$, and controls $\Delta = (\Delta_a)_{a \in A_{\text{act}}}$. In the context of gas networks with horizontal pipes, potentials represent squared gas pressures at the nodes, i.e., $\pi_u = p_u^2$ for $u \in V$. We note that potential-based flow models are also capable of handling non-horizontal pipes; see Gross et al. (2019). For modeling active elements, a variety of different modeling approaches exist that range from simple linear to sophisticated mixed-integer nonlinear ones; see Fügenschuh et al. (2015). In this paper, we focus on linearly modeled active elements similar to Aßmann (2019). A compressor or control valve $a \in A_{\text{act}}$ linearly increases, respectively decreases, potentials by $\Delta_a \in [0, \Delta_a^+]$, where $\Delta_a^+ \geq 0$ is an upper bound on its capability to increase or decrease the potential. The compressor or control valve can only be active if a minimal quantity of flow passes the arc in the "correct" direction, i.e., if $q_a > m_a$ holds for some given threshold value $m_a \geq 0$. We model an active element $a = (u, v) \in A_{\text{act}}$ by

$$\pi_u - \pi_v = \begin{cases} -\Delta_a, & \text{if } a \in A_{\text{cm}}, \\ \Delta_a, & \text{if } a \in A_{\text{cv}}, \end{cases}$$
$$\Delta_a \in [0, \Delta_a^+ \chi_a(q)],$$

where the indicator function $\chi_a(q)$ is given by

$$\chi_a(q) := \begin{cases} 1, & \text{if } q_a > m_a, \\ 0, & \text{otherwise.} \end{cases}$$

We note that modeling the indicator function χ_a introduces binary variables in general, which we explicitly consider in Sect. 4. We can now formally define the feasibility of a nomination and a booking.

Definition 2.4 A nomination $\ell \in N$ is *feasible* if (q, π, Δ) exists that satisfies

$$\sum_{a \in \delta^{\text{out}}(u)} q_a - \sum_{a \in \delta^{\text{in}}(u)} q_a = \begin{cases} \ell_u, & u \in V_+, \\ -\ell_u, & u \in V_-, \\ 0, & u \in V_0, \end{cases} \tag{1a}$$

$$\pi_u - \pi_v = \Lambda_a q_a |q_a|, \quad a = (u, v) \in A_{\text{pipe}}, \tag{1b}$$

$$\pi_u - \pi_v = \begin{cases} -\Delta_a, & a = (u, v) \in A_{\text{cm}}, \\ \Delta_a, & a = (u, v) \in A_{\text{cv}}, \end{cases} \tag{1c}$$

$$\Delta_a \in [0, \Delta_a^+ \chi_a(q)], \quad a \in A_{\text{act}}, \tag{1d}$$

$$\pi_u \in [\pi_u^-, \pi_u^+], \quad u \in V, \tag{1e}$$

where $\delta^{\text{out}}(u)$ and $\delta^{\text{in}}(u)$ denote the sets of arcs leaving and entering node $u \in V$, $\Lambda_a > 0$ is a pipe-specific potential drop coefficient for all $a \in A_{\text{pipe}}$, $0 < \pi_u^- \leq \pi_u^+$ are potential bounds for all $u \in V$, and $0 \leq \Delta_a^+$ is an upper bound on the operation of each active element $a \in A_{\text{act}}$.

Constraints (1a) ensure flow conservation at every node of the network. For pipes $a \in A_{\text{pipe}}$, Constraints (1b) link the arc flow to the incident node potentials. For active elements $a \in A_{\text{act}}$, Constraints (1c) determine the potentials incident to the active element according to its control Δ_a. Moreover, Constraints (1d) ensure that the active elements operate in the allowed ranges, which are due to technical restrictions. Finally, the potentials have to satisfy certain potential bounds, see Constraints (1e). The feasibility of a booking is then defined as follows.

Definition 2.5 A booking $b \in L$ is *feasible* if all booking-compliant nominations $\ell \in N(b)$ are feasible, i.e., a booking b is feasible if

$$\forall \ell \in N(b) \; \exists (q, \pi, \Delta) \text{ satisfying (1).} \tag{2}$$

Consequently, for checking the feasibility of a booking, possibly infinitely many booking-compliant nominations have to be checked for feasibility.

From a robust optimization perspective, Problem (2) can be seen as a special two-stage robust or adjustable robust optimization problem, see Ben-Tal et al. (2009); Yanıkoğlu et al. (2019) for more details. Here, the uncertainty set consists of all booking-compliant nominations $N(b)$. Moreover, the robust problem consists only of so-called "wait-and-see" decisions given by (1) and no "here-and-now" decisions are made. The switch from passive to active networks makes Problem (2) even more challenging since it introduces binary "wait-and-see" decisions due to the indicator functions χ_a for all $a \in A_{\text{act}}$.

3 Why active elements are difficult

In this section, we first review a known characterization of the feasibility of a booking in passive networks as obtained in Labbé et al. (2020). Afterward, we show that this characterization cannot be applied to the considered case with active elements, which illustrates the need for new methods to decide the feasibility of a booking in active networks.

In passive networks, the feasibility of a given booking b can be characterized by computing the maximum potential difference for each pair of nodes; see Theorem 10 in Labbé et al. (2020). For each pair of nodes $(w_1, w_2) \in V^2$, the authors introduce the nonlinear optimization problem

$$\varphi_{w_1 w_2}(b) := \max_{\ell, q, \pi} \quad \pi_{w_1} - \pi_{w_2} \tag{3a}$$

$$\text{s.t.} \quad \sum_{a \in \delta^{\text{out}}(u)} q_a - \sum_{a \in \delta^{\text{in}}(u)} q_a = \begin{cases} \ell_u, & u \in V_+, \\ -\ell_u, & u \in V_-, \\ 0, & u \in V_0, \end{cases} \tag{3b}$$

$$\pi_u - \pi_v = \Lambda_a q_a |q_a|, \quad a = (u, v) \in A, \tag{3c}$$

$$0 \leq \ell_u \leq b_u, \quad u \in V. \tag{3d}$$

The feasibility of a booking is then characterized by constraints on the optimal value $\varphi_{w_1 w_2}(b)$ of (3).

Theorem 3.1 (Theorem 10 in Labbé et al. (2020)) *Let $G = (V, A)$ be a weakly connected and passive network and let $b \in L$ be a booking. Then, the booking b is feasible if and only if for each pair of nodes $(w_1, w_2) \in V^2$, the corresponding optimal value $\varphi_{w_1 w_2}(b)$ satisfies*

$$\varphi_{w_1 w_2}(b) \leq \pi^+_{w_1} - \pi^-_{w_2}. \tag{4}$$

For passive tree-shaped or passive single-cycle networks, this characterization can be checked in polynomial time; see Labbé et al. (2020, 2021); Robinius et al. (2019). However, the problem of validating a booking on general passive networks is known to be coNP-hard (Thürauf 2020).

Unfortunately, the characterization given in Theorem 3.1 does not hold if active elements are present in the network, which we demonstrate by the following counterexample. To this end, we consider a tree $G = (V, A)$ with corresponding lower and upper potential bounds π^- and π^+:

$$V := \{s, v, t\}, \quad A := \{(s, v), (v, t)\},$$
$$\pi^-_s = \pi^+_s = 5, \quad \pi^-_v = 0, \ \pi^+_v = 10, \quad \pi^-_t = 5, \ \pi^+_t = 7,$$

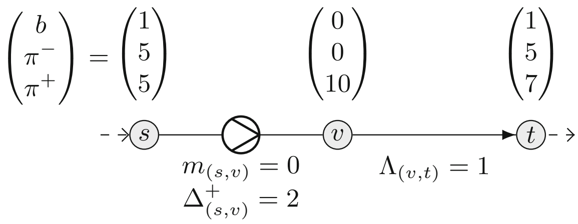

Fig. 1 Network of the counterexample consisting of three nodes, one compressor, and one pipe, together with relevant node and arc parameters

where $s \in V_+$ is an entry node, $t \in V_-$ is an exit node, and $v \in V_0$ is an inner node. Furthermore, $(s, v) \in A_{\text{cm}}$ is a compressor that operates in the range $\Delta_{(s,v)} \in [0, 2]$ if $q_{(s,v)} > m_{(s,v)} = 0$ and otherwise, it is switched to bypass mode, i.e., $\Delta_{(s,v)} = 0$. The arc $(v, t) \in A_{\text{pipe}}$ is a pipe with potential drop coefficient $\Lambda_{(v,t)} = 1$. A graphical representation is given in Figure 1.

We consider the booking $(b_s, b_v, b_t) = (1, 0, 1)$. By construction, every feasible point of (3) satisfies $0 \leq q_a \leq 1$ for all $a \in A$. To apply the passive characterization (4) to the active network $G = (V, A)$, we set the active element to bypass mode and interpret it as a pipe with $\Lambda_{(s,v)} = 0$. Consequently, it follows that the characterization conditions (4) are directly satisfied for every pair of nodes except of (s, t). For the latter pair of nodes, the booking-compliant nomination $(\ell_s, \ell_v, \ell_t) = (1, 0, 1)$ is the optimal solution of (3) w.r.t. (s, t) with objective value $\varphi_{st}(b) = 1$ and therefore violates the corresponding condition (4). Consequently, the booking is infeasible. However, this is not correct here since the compressor can be used to compensate the potential loss. In particular, for every booking-compliant nomination $\ell \in N(b)$, we can explicitly construct a corresponding feasible point of (1) as follows: The zero nomination is feasible due to $\pi_u = 5$ for all $u \in V$, $q_a = 0$ for all $a \in A$, $\Delta_{(s,v)} = 0$, and $\chi_{(s,v)}(q) = 0$. Thus, we now consider an arbitrary nonzero nomination $\ell \in N(b)$. The corresponding flows q are unique since G is a tree. We thus can construct the following feasible point of (1):

$$\pi_s = 5,\ \pi_v = 7,\ \pi_t = 7 - q_{(v,t)}^2, \quad \Delta_{(s,t)} = 2,\ \chi_{(s,v)}(q) = 1,$$

where $\pi_t = 7 - q_{(v,t)}^2 \in [5, 7]$ holds due to $0 \leq q_a \leq 1$ for all $a \in A$. This small counterexample illustrates that the existing characterization for deciding the feasibility of a booking in passive networks cannot be applied directly to the case of networks with active elements.

Furthermore, the introduction of active elements may lead to a disconnected set of feasible nominations, which is proven to be connected for the case of passive networks; see Schewe et al. (2020). We can observe this effect in our small counterexample by setting the threshold value $m_{(s,v)} = 0.5$. Then, the set of nominations $N(b)$ splits into infeasible nominations $\{(\ell_s, \ell_v, \ell_t) = (x, 0, x) \colon x \in (0, 0.5]\}$ and the set of feasible nominations $\{(\ell_s, \ell_v, \ell_t) = (x, 0, x) \colon x \in (0.5, 1]\} \cup \{(0, 0, 0)\}$, which are not connected. Consequently, the booking $(b_s, b_v, b_t) = (1, 0, 1)$ is infeasible. We additionally note that the maximum potential difference between s and t is 0.25, which is obtained by the nomination (0.5, 0, 0.5) that differs from the optimal solution $\varphi_{st}(b)$ given by (1, 0, 1) of the passive characterization (4). Consequently, the usual monotonicity property of passive network, namely that more flow between a pair of nodes leads to a larger potential difference, is not satisfied in active networks anymore.

In the following section, we adapt the method of computing maximum potential differences to decide the feasibility of a booking in active networks using a bilevel approach. Choosing the tool of bilevel optimization is based on the following intuition. First, an arbitrary booking-compliant nomination is chosen. Afterward, the TSO controls the active elements to transport the nomination through the network. If this is possible for every booking-compliant nomination, then the booking is feasible. Otherwise, it is infeasible. We explore this bilevel perspective to derive new methods to decide the feasibility of a booking in networks with active elements.

4 Bilevel modeling

We adapt the methodology of Labbé et al. (2020) to validate a booking on networks with active elements by adequately computing nominations with maximum potential difference. As previously discussed, an analogous single-level optimization problem is not sufficient if active elements are present. Here, we consider a max-min bilevel optimization problem. The leader chooses a booking-compliant nomination $\ell \in N(b)$ that maximally violates potential bounds. The goal of the follower, i.e., the TSO, is to transport this nomination while minimizing the violation. The TSO determines flows q, potentials π, and controls Δ of the active elements according to (1), where the potential bound intervals are adjusted using auxiliary variables $y, z \in \mathbb{R}$. More precisely, for every node $u \in V$ it is required that $\pi_u \in [\pi_u^- - y, \pi_u^+ + z]$. The bilevel problem is thus given by

$$\sup_{\ell \in N(b)} \min_{q, \pi, \Delta, y, z} \quad y + z \tag{5a}$$

$$\text{s.t.} \quad \text{(1a)–(1d)},$$

$$\pi_u + y \geq \pi_u^-, \quad u \in V, \tag{5b}$$

$$\pi_u - z \leq \pi_u^+, \quad u \in V. \tag{5c}$$

In this bilevel model, we use "sup" instead of "max" in the upper level, since bilevel-optimal solutions might not be attainable. In fact, the bilevel-feasible region may not be closed in the presence of continuous linking variables, i.e., of variables of the upper level that appear in the lower level, and integer decisions at the lower level; see Moore and Bard (1990); Vicente et al. (1996); Köppe et al. (2010). In (5), the linking variables are given by the nomination ℓ and the binary decisions of the lower level are induced by the indicator functions χ_a for all $a \in A_{\text{act}}$. However, we observe in the following that under the structural assumption 1 considered in this paper, the supremum is indeed attained.

In Problem (5), the leader chooses a booking-compliant nomination and maximizes the sum of the violation $y \in \mathbb{R}$ of lower potential bounds and the violation $z \in \mathbb{R}$ of upper potential bounds. The follower transports the nomination through the network and chooses a control of the active elements to minimize the total potential bound violation, as modeled by (5b) and (5c). This max-min problem, where leader and follower share the same objective function, is part of a special class of bilevel optimization problems, which includes, e.g., interdiction-like problems; see Wood (2011); Smith and Song (2020) and Section 6 of Kleinert et al. (2021). If the optimal value of (5) is positive, then there exists an infeasible nomination. In this case, the leader has chosen a nomination such that the follower cannot route flows without violating the potential bounds. In contrast, if the optimal value is nonpositive, then the corresponding booking is feasible. From the perspective of the TSO, this objective value measures how close within or how far outside of its physical capabilities the network is operated given a "worst-case" nomination w.r.t. the considered booking. The following result proves the correctness of Problem (5).

Proposition 4.1 *Let $G = (V, A)$ be a weakly connected network with linearly modeled active elements $A_{\text{act}} \subseteq A$. Then, the booking $b \in L$ is feasible if and only if the optimal value of (5) is nonpositive.*

Proof If the optimal value of (5) is positive, it is clear that there exists a bilevel-feasible point (ℓ, q, π, y, z) such that the nomination ℓ violates either a lower potential bound $(y > 0)$ or an upper potential bound $(z > 0)$. Thus, the booking is infeasible in that case.

Suppose now that for every feasible point $(\ell, q, \pi, \Delta, y, z)$ of (5), it holds that $y + z \leq 0$. If $y, z \leq 0$, all booking-compliant nominations can be transported within the original potential bounds and the booking is feasible. If $y > 0$ and $z \leq -y$, the nomination ℓ violates at least one lower potential bound $\pi_u = \pi_u^- - y < \pi_u^-$ for $u \in V$. Without changing flows q or the controls Δ, we consider new potentials $\tilde{\pi}_u := \pi_u + y$ for all $u \in V$. Adapting the corresponding auxiliary variables $\tilde{y} := 0$ and $\tilde{z} := y + z \leq 0$, we have constructed a new solution $(\ell, q, \tilde{\pi}, \Delta, \tilde{y}, \tilde{z})$ of the same objective value without any violation of lower or upper potential bounds. The symmetric case of $z > 0$ and $y \leq -z$ can be treated analogously. □

It has been discussed in Sect. 3 that the problem of validating the feasibility of a booking when considering active elements is difficult in general. This is reflected in Problem (5), which is a bilevel problem with nonlinear and nonconvex lower level and for which optimal solutions may not be attainable. Thus, to tackle this highly challenging problem we need to make the following structural assumption that allows us to derive a practically more tractable reformulation of the bilevel model considered so far.

Assumption 1 No active element is part of an undirected cycle in G.

We note that this assumption is also used in Aßmann et al. (2019); Aßmann (2019). Figure 2 shows on the left a stylized gas network satisfying Assumption 1. Intuitively, Assumption 1 implies that there cannot be any flow along a cycle in the network. More precisely, flow in pipes always leads to a potential drop due to (1b), which for flows along a cycle would lead to mismatching starting and end potentials on that cycle. Such a mismatch could however be fixed by using active elements that act on that cycle in order to match starting and end potentials. Assumption 1 eliminates this possibility and allows us to show the uniqueness of the flows corresponding to any given nomination. To this end, we extend the results of Maugis (1977); Collins et al. (1978); Ríos-Mercado et al. (2002) for passive networks.

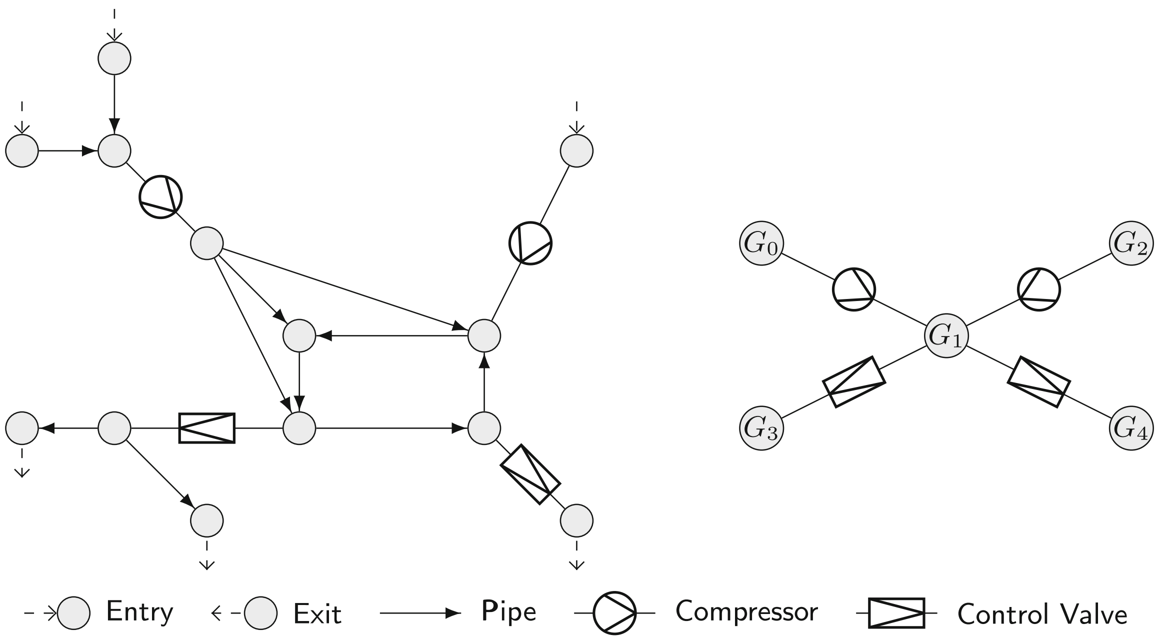

Fig. 2 Stylized gas network satisfying Assumption 1 (left) and its reduced network (right)

Theorem 4.2 *Suppose that Assumption 1 holds. Then, for a given nomination $\ell \in N$, every feasible point (q, π) of (1a) and (1b) admits the same unique flows q_a for all $a \in A$ and the same unique potential differences $\pi_u - \pi_v$ for all $(u, v) \in A_{\text{pipe}}$.*

Proof We prove that flows q are uniquely determined by the nomination ℓ. The uniqueness of potential differences on pipes then directly follows from (1b). First, observe that by Assumption 1, the removal of an active element $a \in A_{\text{act}}$ decomposes the network $G = (V, A)$ into two smaller networks. Moreover, after removing all active elements A_{act}, the network G is split into disconnected and passive components.

If $A_{\text{act}} = \emptyset$, the network G is passive and the result follows from Maugis (1977); Collins et al. (1978). By induction on $|A_{\text{act}}|$, we show that the result also holds true in general. Thus, suppose that the result holds for networks with at most $|A_{\text{act}}| - 1$ active elements. We remove an arbitrary active element $a \in A_{\text{act}}$ from G, which results in two networks with fewer active elements $G_1 = (V_1, A_1)$ and $G_2 = (V_2, A_2)$. We assume w.l.o.g. that $a = (s, t)$ with $s \in V_1$ and $t \in V_2$. For every node $u \in V$, we define

$$\sigma_u := \begin{cases} 1, & \text{if } u \in V_+, \\ -1, & \text{if } u \in V_-, \\ 0, & \text{if } u \in V_0. \end{cases}$$

Then, the balancedness of supply and demand of nomination ℓ implies that the arc flow q_a is uniquely given by

$$q_a = \sum_{u \in V_1} \sigma_u \ell_u = - \sum_{u \in V_2} \sigma_u \ell_u.$$

Starting from the nomination ℓ, we now construct another nomination $\tilde{\ell}$ for G_1 that is balanced over V_1. We define $\tilde{\ell}_u := \ell_u$ for all $u \in V_1 \setminus \{s\}$ and

$$\tilde{\ell}_s := \left| \sigma_s \ell_s - \sum_{w \in V_1} \sigma_w \ell_w \right|.$$

All nodes in $V_1 \setminus \{s\}$ keep the same nomination value. The modification at node s might change its role, i.e., it can either be an entry, an exit, or an inner node. Thus, we also define $\tilde{\sigma}_u := \sigma_u$ for all $u \in V_1 \setminus \{s\}$ and

$$\tilde{\sigma}_s := \begin{cases} 1, & \text{if } \sigma_s \ell_s - \sum_{w \in V_1} \sigma_w \ell_w > 0, \\ -1, & \text{if } \sigma_s \ell_s - \sum_{w \in V_1} \sigma_w \ell_w < 0, \\ 0, & \text{if } \sigma_s \ell_s - \sum_{w \in V_1} \sigma_w \ell_w = 0, \end{cases}$$

which exactly corresponds to the sign of $\sigma_s \ell_s - \sum_{w \in V_1} \sigma_w \ell_w$. In particular, we have produced a nomination for G_1, since

$$\sum_{u \in V_1} \tilde{\sigma}_u \tilde{\ell}_u = \sum_{u \in V_1 \setminus \{s\}} \sigma_u \ell_u + \sigma_s \ell_s - \sum_{w \in V_1} \sigma_w \ell_w = 0.$$

By the induction hypothesis, the restriction of q to A_1 is uniquely determined. Symmetrical arguments can be applied to show that the restriction of q to A_2 is also unique. Finally, the result follows given the fact that $A = A_1 \cup A_2 \cup \{a\}$. □

The latter result implies that, once a nomination is given, most lower-level decisions in (5) are already fixed by physics. The lower-level problem can thus be reduced to only include the remaining decision variables. Therefore, consider the collection of passive subnetworks obtained by removing all active elements from G, which we denote by $\mathcal{G} := \{G_0, G_1, \ldots, G_{|A_{\text{act}}|}\}$. For convenience, we sometimes denote an active arc $a \in A_{\text{act}}$ by $a = (G_i, G_j)$ if $a = (u, v)$ for $u \in V(G_i)$ and $v \in V(G_j)$. Then, by Assumption 1, the graph $\tilde{G} = (\mathcal{G}, A_{\text{act}})$ obtained by merging passive subnetworks into single nodes is a tree. In line with Ríos-Mercado and Borraz-Sánchez (2015); Ríos-Mercado et al. (2002), we call $\tilde{G}$ the *reduced network*. Figure 2 illustrates a network (left) and its associated reduced network (right).

Using the rationale of Ríos-Mercado et al. (2002), it follows by Theorem 4.2 that the potentials corresponding to a nomination $\ell \in N$ are determined as soon as a reference potential in an arbitrary passive subnetwork $G_j \in \mathcal{G}$ and the controls Δ_a of all active elements $a \in A_{\text{act}}$ are fixed. Exploiting this uniqueness of flows and potentials, the following result presents an equivalent reformulation of Problem (5). Therein, the upper level consists of a potential-based flow over G where all active elements are inactive, i.e., $\pi_u = \pi_v$ for all $(u, v) \in A_{\text{act}}$. The TSO then reacts by using the active elements, as well as a constant shift τ_j to be applied to the potentials of all the nodes $u \in V(G_j)$ for every passive subnetwork $G_j \in \mathcal{G}$. Intuitively, in addition to choosing a worst-case nomination, the upper-level player thus already fixes all physical quantities that are uniquely determined by the nomination, i.e., all flows and the potential differences on pipes. The lower level, on the other hand, consists of a problem containing only those decision variables that the TSO influences. In addition, this new bilevel structure allows us to linearly model the indicator function χ_a for the activation of an element $a \in A_{\text{act}}$ using binary variables.

Theorem 4.3 *Consider the bilevel problem*

$$\max_{\ell,q,\pi,s} \quad y+z \tag{6a}$$
$$\text{s.t.} \quad (1a), (1b), \tag{6b}$$
$$\ell \in N(b), \tag{6c}$$
$$\pi_u = \pi_v, \quad (u,v) \in A_{\text{act}}, \tag{6d}$$
$$q_a \le m_a(1-s_a) + Ms_a, \quad a \in A_{\text{act}}, \tag{6e}$$
$$s_a \in \{0,1\}, \quad a \in A_{\text{act}}, \tag{6f}$$
$$(\Delta, \tau, y, z) \in \mathcal{R}(\ell, q, \pi, s), \tag{6g}$$

where $M := \min\{\sum_{u\in V_+} b_u, \sum_{u\in V_-} b_u\}$ *is an upper bound on the flow on any arc and the set of lower-level solutions* $\mathcal{R}(\ell,q,\pi,s)$ *is given by*

$$\operatorname*{arg\,min}_{\Delta,\tau,y,z} \quad y+z \tag{7a}$$
$$\text{s.t.} \quad \tau_i - \tau_j = \begin{cases} -\Delta_a, & a = (G_i, G_j) \in A_{\text{cm}}, \\ \Delta_a, & a = (G_i, G_j) \in A_{\text{cv}}, \end{cases} \tag{7b}$$
$$\Delta_a \in [0, \Delta_a^+ s_a], \quad a \in A_{\text{act}}, \tag{7c}$$
$$\tau_j + y \ge \pi_u^- - \pi_u, \quad u \in V(G_j),\ G_j \in \mathcal{G}, \tag{7d}$$
$$\tau_j - z \le \pi_u^+ - \pi_u, \quad u \in V(G_j),\ G_j \in \mathcal{G}. \tag{7e}$$

Under Assumption 1, Problems (5) and (6) admit the same optimal value.

Proof Let $(\ell, q, \pi, \Delta, y, z)$ be a bilevel-feasible point of (5). In Ríos-Mercado et al. (2002), it is shown that for a passive network, all potentials are uniquely determined once a reference potential is fixed. In particular, all solutions of (1a) and (1b) are equivalent up to a constant shift in every passive subnetwork. Thus, potentials in every passive subnetwork $G_j \in \mathcal{G}$ are of the form $\pi_u = \pi_u(\ell) + \tau_j$ for all $u \in V(G_j)$, where $\pi(\ell)$ is a solution of (1b) and (6d). Moreover, $\tau_j \in \mathbb{R}$ is an arbitrary shift of the potentials in G_j. Constraints (7b) then also hold, since the potentials π satisfy (1c). It remains to model the indicator function χ. For every $a \in A_{\text{act}}$, we set $s_a = 1$ if and only if $q_a > m_a$. Since $q_a \le M$, it follows that (6e) is satisfied. Consequently, $(\ell, q, \pi(\ell), s, \Delta, \tau, y, z)$ is bilevel feasible for (6) and admits the same objective value.

For the converse, first note that for every $a \in A_{\text{act}}$, Constraints (6e) guarantee that $s_a = 1$ holds if $q_a > m_a$. Assume now that $q_a \le m_a$. Then, the leader's decision on s_a is arbitrary. However, the lower level with $s_a = 1$ is a relaxation of the lower level with $s_a = 0$. Upper and lower level have the same objective function with opposing optimization directions. Consequently, there is a bilevel-optimal solution of (6) with $s_a = 0$, and thus satisfying $s_a = \chi_a(q)$. Let $(\ell, q, \pi, s, \Delta, \tau, y, z)$ be a bilevel-optimal solution of (6) with $s_a = \chi_a(q)$ for all $a \in A_{\text{act}}$. Theorem 4.2 states that the flows q corresponding to ℓ and solving the System (1a) and (1b) are unique. If we denote these unique flows by $q(\ell)$, then $q = q(\ell)$ and every bilevel-feasible point of (5) also admits flows $q(\ell)$. Let us now define $\tilde{\pi}_u := \pi_u + \tau_j$ for all $u \in V(G_j)$ and $G_j \in \mathcal{G}$. Then, $(\ell, q, \tilde{\pi}, \Delta, y, z)$ is bilevel-feasible for (5) and admits the same objective function value. □

Since the integer decisions are at the upper level of Problem (6) and all variables of the lower level (7) are continuous, all bilevel-optimal solutions are indeed attained, which allows us to use “max” in (6). As a consequence of Theorem 4.3, the optimal solution of (5) is then attained under Assumption 1 as well. Hence, in this case, the “sup” in (5) can be replaced by a “max”.

To summarize, in this section we first presented a bilevel optimization model of the adversarial interplay of checking the feasibility of a booking. In the resulting Problem (5), the upper-level player selects the worst possible nomination w.r.t. a violation of the potential bounds. The lower-level player, i.e., the TSO, determines flows, potentials, and a control of the active elements to minimize the violation. Exploiting the structure resulting from Assumption 1, we deduced that many of the physical quantities of the TSO’s problem are already uniquely determined by the upper-level nomination. These observations led to Problem (6), where only variables that the TSO can actively control remain in the lower-level problem. Moving flow and potential variables to the upper level has, in particular, allowed us to linearly model the indicator functions χ. Note also that in Problem (6), the upper level is a mixed-integer nonlinear problem (MINLP), but the lower level is a linear problem (LP) for fixed upper-level decisions. In the next section, we will focus on Problem (6) and derive the classical KKT reformulation.

5 Karush–Kuhn–Tucker reformulation

Problem (6) is a bilevel problem with mixed-integer variables. In general, these problems are strongly NP-hard, see, e.g., Hansen et al. (1992). Many approaches for bilevel problems with mixed-integer variables rely on the fact that the linking variables, i.e., the variables of the upper level that appear in the lower level, are all integers. This is not the case here since, in addition to the binaries s_a for $a \in A_{\text{act}}$, the potentials π_u for $u \in V$ link the upper and the lower level. However, we observe that the lower level of (6) is linear for every fixed upper-level decision. As a consequence, we can characterize the optimal solutions of the lower level using its KKT conditions.

5.1 Reformulation

Let us first consider the lower level’s dual problem for a fixed upper-level decision (ℓ, q, π, s). We introduce dual variables α_a for $a \in A_{\text{act}}$ for constraints (7b), δ_u^- and δ_u^+ for $u \in V$ corresponding to (7d) and (7e), and finally β_a for $a \in A_{\text{act}}$ associated to the upper bound on Δ_a. The dual problem is then given by

$$\max_{\alpha,\beta,\delta^+,\delta^-} \quad -\sum_{a\in A_{\text{act}}} \Delta_a^+ s_a \beta_a + \sum_{u\in V} \big((\pi_u^- - \pi_u)\delta_u^- - (\pi_u^+ - \pi_u)\delta_u^+\big) \tag{8a}$$

$$\text{s.t.} \quad \sum_{a\in\delta^{\text{out}}(G_j)} \alpha_a - \sum_{a\in\delta^{\text{in}}(G_j)} \alpha_a = \sum_{u\in V(G_j)} (\delta_u^+ - \delta_u^-), \quad G_j \in \mathcal{G}, \tag{8b}$$

$$\alpha_a \le \beta_a, \ \beta_a \ge 0, \quad a \in A_{\text{cm}}, \tag{8c}$$

$$-\alpha_a \le \beta_a, \ \beta_a \ge 0, \quad a \in A_{\text{cv}}, \tag{8d}$$

$$\sum_{u\in V} \delta_u^+ = 1, \ \sum_{u\in V} \delta_u^- = 1, \tag{8e}$$

$$\delta_u^+, \delta_u^- \ge 0, \quad u \in V. \tag{8f}$$

Let $\tilde{G}$ be the reduced network obtained from G by merging all passive subnetworks. The dual problem (8) can then be interpreted as a flow problem on $\tilde{G}$. From that point of view, α represents dual flows, β are the capacities on arcs corresponding to active elements, and $\sum_{u\in V(G_j)} \delta_u^+$ and $\sum_{u\in V(G_j)} \delta_u^-$ are the supply and demand at each node G_j. Constraints (8b) ensure dual flow balance. Note that the dual arc flows have an unconstrained sign, with the same interpretation as before, i.e., $\alpha_a > 0$ corresponds to flow in the direction of arc $a \in A_{\text{act}}$, while $\alpha_a < 0$ represents flow in the opposite direction. For compressors $a \in A_{\text{cm}}$, dual flows are bounded from above, i.e., flow in the direction of the arc is bounded, whereas for control valves $a \in A_{\text{cv}}$, arc flows are bounded from below, i.e., flow in the opposite direction of the arc is bounded. Finally, total supply and demand equal one; see (8e).

The KKT conditions for the lower level consist of primal feasibility (7b)–(7e), dual feasibility (8b)–(8f), and the complementarity constraints

$$\delta_u^-(\tau_j + y + \pi_u - \pi_u^-) = 0, \quad u \in V(G_j), \ G_j \in \mathcal{G}, \tag{9a}$$

$$\delta_u^+(\tau_j - z + \pi_u - \pi_u^+) = 0, \quad u \in V(G_j), \ G_j \in \mathcal{G}, \tag{9b}$$

$$\beta_a(\Delta_a - \Delta_a^+ s_a) = 0, \quad a \in A_{\text{act}}, \tag{9c}$$

$$(-\alpha_a + \beta_a)\Delta_a = 0, \quad a \in A_{\text{cm}}, \tag{9d}$$

$$(\alpha_a + \beta_a)\Delta_a = 0, \quad a \in A_{\text{cv}}. \tag{9e}$$

Consequently, Problem (6) can be reformulated as the MINLP

$$\max_{\xi} \quad y + z \tag{10}$$

$$\text{s.t.} \quad \text{(6b)–(6f)}, \tag{UL}$$

$$\text{(7b)–(7e)}, \tag{LLP}$$

$$\text{(8b)–(8f)}, \tag{LLD}$$

$$\text{(9)},$$

where $\xi = (\ell, q, \pi, s, \Delta, \tau, y, z, \alpha, \beta, \delta^+, \delta^-)$ is the vector of upper-level, lower-level primal, and lower-level dual variables. Here, Constraint (UL) groups all upper-level constraints. Constraint (LLP) and Constraint (LLD) group lower-level primal and dual constraints, respectively.

5.2 Big-M linearization

A standard way of reformulating the KKT complementarity conditions (9) is via big-M linearizations; see Fortuny-Amat and McCarl (1981). For a dual variable $\lambda \geq 0$ and a primal constraint $c(x) \geq 0$, the complementarity condition $\lambda c(x) = 0$ is replaced by

$$\lambda \leq M_{\mathrm{d}} u, \quad c(x) \leq M_{\mathrm{p}}(1-u),$$

where $u \in \{0, 1\}$ is an auxiliary binary variable and $M_{\mathrm{d}}, M_{\mathrm{p}} \geq 0$ are upper bounds for λ and $c(x)$, respectively. It is shown in Kleinert et al. (2020) that determining a bilevel-correct big-M is a hard task if problem-specific knowledge is lacking. In the following, by exploiting the structure of Problem (6), we obtain provably correct bounds on lower-level primal and dual variables that can be used for a linearization of (9). First, let us consider the lower-level's dual variables.

Lemma 5.1 *Let (ℓ, q, π, s) be feasible for (UL). Then, there is a corresponding optimal solution $(\alpha, \beta, \delta^+, \delta^-)$ of the lower level's dual problem (8) with $\alpha_a \in [-1, 1]$ and $\beta_a \in [0, 1]$ for all $a \in A_{\mathrm{act}}$ as well as $\delta_u^+, \delta_u^- \in [0, 1]$ for all $u \in V$.*

Proof If follows directly from (8e) and (8f) that $\delta_u^+, \delta_u^- \in [0, 1]$ holds for all $u \in V$. Following the interpretation of the lower level's dual problem as a flow problem on $\tilde{G}$, it holds that $|\alpha_a| \leq 1$ for all $a \in A_{\mathrm{act}}$, since the total demand and supply are both 1 and $\tilde{G}$ is a tree under Assumption 1. Finally, by optimality it follows that $\beta_a \leq 1$ holds if for an arc $a \in A_{\mathrm{act}}$ the inequality $\Delta_a^+ s_a > 0$ is satisfied. Otherwise, if $\Delta_a^+ s_a = 0$ holds for an arc $a \in A_{\mathrm{act}}$, then β_a can be chosen arbitrarily in $[0, 1]$. □

Next, we derive bounds for lower-level primal variables such that an optimal solution satisfying them always exists.

Lemma 5.2 *Let $(\ell, q, \pi, s, \Delta, \tau, y, z)$ be a bilevel-feasible point of (6), then for any $\tilde{\varepsilon}, \varepsilon \in \mathbb{R}$, the point $(\ell, q, \pi + \tilde{\varepsilon}, s, \Delta, \tau + \varepsilon, y - \varepsilon - \tilde{\varepsilon}, z + \varepsilon + \tilde{\varepsilon})$ is also bilevel feasible with the same objective value.*

Proof Let $(\ell, q, \pi, s, \Delta, \tau, y, z)$ be a bilevel-feasible point of (6) and consider arbitrary but fixed $\tilde{\varepsilon}, \varepsilon \in \mathbb{R}$. We now check the feasibility of the point $(\ell, q, \pi + \tilde{\varepsilon}, s, \Delta, \tau + \varepsilon, y - \varepsilon - \tilde{\varepsilon}, z + \varepsilon + \tilde{\varepsilon})$ for (6).

Since we have not changed the upper-level variables ℓ, q, and s, and have only shifted the potential π by $\tilde{\varepsilon}$, upper-level feasibility follows from Theorem 7.1 in (Koch et al. 2015, Chapter 7). We now turn to the lower level. Since the lower-level variables Δ stay unchanged, Constraint (7c) holds. Moreover, Constraints (7b), (7d), and (7e) are satisfied due to

$$\tau_i + \varepsilon - \tau_j - \varepsilon + \omega_a \Delta_a = \tau_i - \tau_j + \omega_a \Delta_a = 0, \qquad a = (G_i, G_j) \in A_{\mathrm{act}},$$
$$\tau_j + \varepsilon + y - \varepsilon - \tilde{\varepsilon} = \tau_j + y - \tilde{\varepsilon} \geq \pi_u^- - \pi_u - \tilde{\varepsilon}, \qquad u \in V(G_j),\ G_j \in \mathcal{G},$$
$$\tau_j + \varepsilon - z - \varepsilon - \tilde{\varepsilon} = \tau_j - z - \tilde{\varepsilon} \leq \pi_u^+ - \pi_u - \tilde{\varepsilon}, \qquad u \in V(G_j),\ G_j \in \mathcal{G}.$$

This shows the feasibility of the considered point. Additionally, the objective values of both points are equal, which directly follows by construction. □

Corollary 5.3 *There is an optimal solution* $(\ell, q, \pi, s, \Delta, \tau, y, z)$ *of (6) that satisfies*

$$\min_{u \in V} \{\pi_u\} = 0 \quad \textit{and} \quad \min_{G_j \in \mathcal{G}} \{\tau_j\} = 0.$$

Using this result, we can bound the values π and τ in an optimal solution.

Lemma 5.4 *There is an optimal solution* $(\ell, q, \pi, s, \Delta, \tau, y, z)$ *of the bilevel problem (6) that satisfies*

$$0 \leq \pi_u \leq \sum_{a \in A} \Lambda_a M^2, \quad u \in V,$$
$$0 \leq \tau_j \leq \sum_{a \in A_{\mathrm{act}}} \Delta_a^+, \quad G_j \in \mathcal{G},$$

where $M := \min\{\sum_{u \in V_+} b_u, \sum_{u \in V_-} b_u\}$ *is an upper bound on the flow on any arc.*

Proof Corollary 5.3 implies that there is an optimal solution $(\ell, q, \pi, s, \Delta, \tau, y, z)$ of the bilevel problem (6) with $u \in V$ and $G_j \in \mathcal{G}$ that satisfies

$$\min_{v \in V} \{\pi_v\} = \pi_u = 0, \quad \min_{G_i \in \mathcal{G}} \{\tau_i\} = \tau_j = 0. \tag{11}$$

For an arbitrary node $v \in V$, we now consider a path $P(u, v)$, which consists of the arcs $A(P(u, v)) \subseteq A$ corresponding to an undirected path from u to v in G. Additionally, for an arc $a = (s, t) \in A(P(u, v))$, we introduce $\eta_a(P)$, which evaluates to 1, if a is directed from u to v, and otherwise it evaluates to -1. Consequently, Constraint (1b) and Condition (11) imply

$$0 \leq \pi_v = \pi_u - \sum_{a \in P(u,v) \cap A_{\mathrm{pipe}}} \eta_a(P) \Lambda_a |q_a| q_a \leq \sum_{a \in A_{\mathrm{pipe}}} \Lambda_a M^2.$$

In analogy, for an arbitrary $G_i \in \mathcal{G}$, Constraints (7b) and Condition (11) imply

$$0 \leq \tau_i = \tau_j + \sum_{a \in P(u,v) \cap A_{\mathrm{cm}}} \eta_a(P) \Delta_a - \sum_{a \in P(u,v) \cap A_{\mathrm{cv}}} \eta_a(P) \Delta_a \leq \sum_{a \in A_{\mathrm{act}}} \Delta_a^+.$$

Finally, it remains to determine big-M bounds for y and z. However, these can be obtained by carefully combining the lower and upper bounds given in Lemma 5.4. It suffices to observe that for a lower-level primal optimal solution, we obtain

$$y = \max_{\substack{G_j \in \mathcal{G},\\ u \in V(G_j)}} \left\{\pi_u^- - \pi_u - \tau_j\right\}, \quad z = \max_{\substack{G_j \in \mathcal{G},\\ u \in V(G_j)}} \left\{\pi_u + \tau_j - \pi_u^+\right\}.$$

6 Optimal-value-function reformulations and characterizations of feasible bookings

As an alternative to the KKT reformulation of Sect. 5, the bilevel problem (6) can also be reformulated using the lower level's optimal value function; see, e.g., Dempe (2002). Let $\varphi(\ell, q, \pi, s)$ be the optimal value of (7) for given upper-level decisions (ℓ, q, π, s). Note that the lower level (7) is feasible for every (ℓ, q, π, s), i.e., (UL) always admits a feasible point. Thus, (6) is equivalent to

$$\max_{\ell,q,\pi,s} \{\varphi(\ell, q, \pi, s) \colon () \text{ UL}). \tag{12}$$

By strong duality of the lower level, φ is also the optimal value function of the lower level's dual problem (8). The latter is a linear problem with objective function parameterized by π and s. Thus, φ is a piecewise-linear and convex function. More precisely, given that the lower level is always feasible and bounded, the same holds for the lower-level's dual problem. The optimal value function φ can thus be expressed as the maximum over the lower level's dual objective function evaluated in a potentially exponential number of vertices of the feasible set of the lower level's dual problem. Consequently, the single-level reformulation (12) is a convex maximization problem over a nonconvex feasible set, which is a highly intractable problem class, in general.

6.1 The optimal value function

We exploit the special structure of the lower level under Assumption 1 to express φ by polynomially many vertices of the polyhedral feasible set of the lower level's dual problem. To this end, let $\tilde{G}$ be the reduced network corresponding to G. Additionally, for every two passive subnetworks $G_i, G_j \in \mathcal{G}$, there exists a unique, undirected path joining them, which we denote by $P(G_i, G_j)$. Choosing any G_k as the root of $\tilde{G}$, we can partition the active elements into arcs pointing away from or towards G_k, i.e., $A_{\text{act}} = A_{\text{act}}^{k,\rightarrow} \cup A_{\text{act}}^{k,\leftarrow}$. Formally, we define

$$A_{\text{act}}^{k,\rightarrow} := \left\{(G_i, G_j) \in A_{\text{act}} \colon P(G_k, G_i) \subseteq P(G_k, G_j)\right\}, \quad A_{\text{act}}^{k,\leftarrow} := A_{\text{act}} \setminus A_{\text{act}}^{k,\rightarrow}.$$

In the following, we prove that for given δ^+ and δ^-, the flow variables α can be uniquely determined using the conservation constraints (8b). Given that (8b) contains $|A_{\text{act}}| + 1$ many linear equations and that the system is of rank $|A_{\text{act}}|$, we can eliminate an arbitrarily chosen row. We denote by G_0 the passive subnetwork in $\mathcal{G}$ for which we delete the corresponding equation in (8b). Then, G_0 can be interpreted as the root of $\tilde{G}$ and we can consider subtrees of $\tilde{G}$ w.r.t. G_0. If we remove an arc $a \in A_{\text{act}}$ in G, then the network decomposes into two subnetworks. For $a \in A_{\text{act}}$ and $G_j \in \mathcal{G}$, the set $\mathcal{G}_a(G_j)$ denotes all passive sub-components that are contained in the subnetwork, which contains G_j after removing arc a. In particular, the subtree of $\tilde{G}$ "following" a is obtained by $\mathcal{G}_a(G_j)$ if $a = (G_i, G_j) \in A_{\text{act}}^{0,\rightarrow}$ and by $\mathcal{G}_a(G_i)$ if $a = (G_i, G_j) \in A_{\text{act}}^{0,\leftarrow}$. The solution of (8b) is then given by the following lemma.

Lemma 6.1 *Constraints (8b) are equivalent to*

$$\alpha_a = -\sum_{G_l \in \mathcal{G}_a(G_j)} \sum_{u \in V(G_l)} \left(\delta_u^+ - \delta_u^-\right), \qquad a = (G_i, G_j) \in A_{\text{act}}^{0,\rightarrow}, \tag{13a}$$

$$\alpha_a = \sum_{G_l \in \mathcal{G}_a(G_i)} \sum_{u \in V(G_l)} \left(\delta_u^+ - \delta_u^-\right), \qquad a = (G_i, G_j) \in A_{\text{act}}^{0,\leftarrow}. \tag{13b}$$

Proof For given supplies δ^+ and demands δ^-, we already noted that α can be interpreted as a flow. Due to Constraints (8e), Constraints (8b), which ensure flow conservation in $\tilde{G}$, always admit feasible flows. For an arc $a = (G_i, G_j) \in A_{\text{act}}^{0,\rightarrow}$, the flow α_a is determined by the net demand

$$D := \sum_{G_l \in \mathcal{G}_a(G_j)} \sum_{u \in V(G_l)} \left(\delta_u^+ - \delta_u^-\right)$$

of the subtree "following" a. If $D \geq 0$, a surplus in supply needs to leave the subtree over a flowing from G_j to G_i. Respecting the sign convention on the flow along directed arcs, it then holds $\alpha_a = -|D| = -D$. If $D < 0$, a surplus in demand needs to be shipped over a into the subtree, thus $\alpha_a = |D| = -D$. Similar arguments apply to $a = (G_i, G_j) \in A_{\text{act}}^{0,\leftarrow}$. □

With this result at hand, we can explicitly determine the vertices of the polyhedral feasible set of the lower level's dual problem (8).

Theorem 6.2 *The vertices of the polyhedron (8) are given by (13) and*

$$\begin{aligned}
\beta_a &= \max\{\alpha_a, 0\}, \quad a \in A_{\text{cm}}, \\
\beta_a &= \max\{-\alpha_a, 0\}, \quad a \in A_{\text{cv}}, \\
\delta_{w_1}^+ &= 1, \ \delta_u^+ = 0, \quad u \in V \setminus \{w_1\}, \\
\delta_{w_2}^- &= 1, \ \delta_u^- = 0, \quad u \in V \setminus \{w_2\},
\end{aligned}$$

for all pairs of nodes $(w_1, w_2) \in V^2$.

Proof By Lemma 6.1, Constraints (13) uniquely determine α as a function of δ^+ and δ^-. Furthermore, for every feasible point of (8), the constraints

$$\begin{aligned}
\beta_a &\geq \max\{\alpha_a, 0\}, \quad a \in A_{\text{cm}}, \\
\beta_a &\geq \max\{-\alpha_a, 0\}, \quad a \in A_{\text{cv}},
\end{aligned}$$

hold and have to be active at a vertex. It is therefore sufficient to determine the vertices of (8e) and (8f) in the space of δ^+ and δ^-, which are given by

$$\begin{aligned} \delta^+_{w_1} = 1,\ \delta^+_u = 0, \quad u \in V \setminus \{w_1\}, \\ \delta^-_{w_2} = 1,\ \delta^-_u = 0, \quad u \in V \setminus \{w_2\}, \end{aligned}$$

for any pair of nodes $(w_1, w_2) \in V^2$. This concludes the proof. □

Using this result and the network structure, we now elaborate on a representation of these vertices as follows. For any two nodes $w_1 \in G_{j_1}$ and $w_2 \in G_{j_2}$, we introduce for any $a = (G_i, G_j) \in A^{0,\rightarrow}_{\text{act}}$,

$$\alpha_a(w_1, w_2) := \begin{cases} -1, & \text{if } G_{j_1} \in \mathcal{G}_a(G_j), G_{j_2} \notin \mathcal{G}_a(G_j), \\ 1, & \text{if } G_{j_1} \notin \mathcal{G}_a(G_j), G_{j_2} \in \mathcal{G}_a(G_j), \\ 0, & \text{otherwise,} \end{cases}$$

and for any $a = (G_i, G_j) \in A^{0,\leftarrow}_{\text{act}}$,

$$\alpha_a(w_1, w_2) := \begin{cases} 1, & \text{if } G_{j_1} \in \mathcal{G}_a(G_i), G_{j_2} \notin \mathcal{G}_a(G_i), \\ -1, & \text{if } G_{j_1} \notin \mathcal{G}_a(G_i), G_{j_2} \in \mathcal{G}_a(G_i), \\ 0, & \text{otherwise.} \end{cases}$$

Furthermore, for any $a \in A_{\text{act}}$, we define

$$\beta_a(w_1, w_2) := \begin{cases} \max\{\alpha_a(w_1, w_2), 0\}, & \text{if } a \in A_{\text{cm}}, \\ \max\{-\alpha_a(w_1, w_2), 0\}, & \text{if } a \in A_{\text{cv}}. \end{cases}$$

Before we give a closed-form expression of the lower-level optimal value function φ, we discuss an alternative way of representing $\alpha_a(w_1, w_2)$ and $\beta_a(w_1, w_2)$. Recall that the set of active elements A_{act} is partitioned into the set of compressors A_{cm} and the set of control valves A_{cv}. The sets $A^{k,\rightarrow}_{\text{act}}$ and $A^{k,\leftarrow}_{\text{act}}$ can be partitioned similarly. For all $a \in A_{\text{act}}$, we then obtain

$$\alpha_a(w_1, w_2) = \begin{cases} -1, & \text{if } a \in P(G_{j_1}, G_{j_2}) \cap A^{j_1,\leftarrow}_{\text{act}}, \\ 1, & \text{if } a \in P(G_{j_1}, G_{j_2}) \cap A^{j_1,\rightarrow}_{\text{act}}, \\ 0, & \text{otherwise.} \end{cases}$$

Consequently, it also holds

$$\beta_a(w_1, w_2) = \begin{cases} 1, & \text{if } a \in P(G_{j_1}, G_{j_2}) \cap \left(A^{j_1,\rightarrow}_{\text{cm}} \cup A^{j_1,\leftarrow}_{\text{cv}}\right), \\ 0, & \text{otherwise.} \end{cases}$$

Using this representation of $\beta_a(w_1, w_2)$, we obtain the closed form of the lower-level optimal value function stated in the following result.

Corollary 6.3 *The optimal value function φ of (7) is given by*

$$\max_{\substack{(G_{j_1},G_{j_2})\in\mathcal{G}^2,\\ w_1\in V(G_{j_1}),\\ w_2\in V(G_{j_2})}} \left\{ \pi_{w_1} - \pi_{w_2} - \left(\pi^+_{w_1} - \pi^-_{w_2} + \sum_{\substack{a\in P(G_{j_1},G_{j_2}):\\ a\in A^{j_1,\rightarrow}_{\mathrm{cm}} \cup A^{j_1,\leftarrow}_{\mathrm{cv}}}} \Delta^+_a s_a \right) \right\}. \tag{14}$$

Similar to the results obtained in Labbé et al. (2020) for passive networks, we can now establish a characterization of feasible bookings for networks (under Assumption 1) with linearly modeled active elements.

Theorem 6.4 *Let $G = (V, A)$ be a weakly connected network satisfying Assumption 1. Then, the booking $b \in L$ is feasible if and only if $\phi_{w_1 w_2}(b) \le \pi^+_{w_1} - \pi^-_{w_2}$ is satisfied for every pair of nodes $(w_1, w_2) \in V^2$ with $w_1 \in V(G_{j_1})$ and $w_2 \in V(G_{j_2})$, where we define*

$$\phi_{w_1 w_2}(b) := \max_{\ell,q,\pi,s} \left\{ \pi_{w_1} - \pi_{w_2} - \sum_{\substack{a\in P(G_{j_1},G_{j_2}):\\ a\in A^{j_1,\rightarrow}_{\mathrm{cm}} \cup A^{j_1,\leftarrow}_{\mathrm{cv}}}} \Delta^+_a s_a : \text{(UL)} \right\}.$$

Proof As a consequence of Proposition 4.1 and Theorem 4.3, the booking b is feasible if and only if the solutions of (12) satisfy $\varphi(\ell, q, \pi, s) \le 0$. By Corollary 6.3, the latter holds if and only if

$$\pi_{w_1} - \pi_{w_2} - \sum_{\substack{a\in P(G_{j_1},G_{j_2}):\\ a\in A^{j_1,\rightarrow}_{\mathrm{cm}} \cup A^{j_1,\leftarrow}_{\mathrm{cv}}}} \Delta^+_a s_a \le \pi^+_{w_1} - \pi^-_{w_2}$$

for every pair of nodes $(w_1, w_2) \in V^2$.

Observe that $\phi_{w_1 w_2}(b) - (\pi^+_{w_1} - \pi^-_{w_2})$ is a lower bound for the solutions of (12). Thus, if the booking is feasible, $\phi_{w_1 w_2}(b) \le \pi^+_{w_1} - \pi^-_{w_2}$ holds for every pair of nodes $(w_1, w_2) \in V^2$. On the contrary, if the booking is infeasible, there exists a feasible point (ℓ, q, π, s) of (UL) and a pair of nodes $(w_1, w_2) \in V^2$ such that $\varphi(\ell, q, \pi, s) > 0$ holds, i.e.,

$$\pi_{w_1} - \pi_{w_2} - \sum_{\substack{a\in P(G_{j_1},G_{j_2}):\\ a\in A^{j_1,\rightarrow}_{\mathrm{cm}} \cup A^{j_1,\leftarrow}_{\mathrm{cv}}}} \Delta^+_a s_a > \pi^+_{w_1} - \pi^-_{w_2}.$$

In particular, we also have $\phi_{w_1 w_2}(b) > \pi^+_{w_1} - \pi^-_{w_2}$. □

The optimal-value-function reformulation (12), where φ is given by (14), requires optimizing a piecewise-linear function with $|V|^2$ pieces over a nonlinear and nonconvex feasible domain. Using the characterization given in Theorem 6.4, all $|V|^2$ linear pieces can be optimized in individual subproblems.

6.2 Reduced optimal value function

Since the lower level mainly controls active elements that link passive subnetworks, it is possible to give a coarser interpretation of the lower-level optimal value function. The main intuition now is to consider the lower level as a problem on the reduced network $\tilde{G}$. By grouping all nodes of a passive subnetwork, we can rewrite the lower-level optimal value function, yielding

$$\max_{(G_{j_1},G_{j_2})\in\mathcal{G}^2} \left\{ \begin{array}{r} \max\limits_{w_1\in V(G_{j_1})} \left\{\pi_{w_1} - \pi_{w_1}^+\right\} + \max\limits_{w_2\in V(G_{j_2})} \left\{\pi_{w_2}^- - \pi_{w_2}\right\} \\ - \sum\limits_{\substack{a\in P(G_{j_1},G_{j_2}):\\ a\in A_{\mathrm{cm}}^{j_1,\rightarrow}\cup A_{\mathrm{cv}}^{j_1,\leftarrow}}} \Delta_a^+ s_a \end{array} \right\}. \tag{15}$$

Then, applying the same arguments as in the proof of Theorem 6.4, we deduce a characterization with fewer subproblems to be solved.

Corollary 6.5 *Let $G=(V,A)$ be a weakly connected network satisfying Assumption 1. Then, the booking $b\in L$ is feasible if and only if $\phi_{j_1j_2}(b)\le 0$ is satisfied for every pair of passive subnetworks $(G_{j_1},G_{j_2})\in\mathcal{G}^2$, where $\phi_{j_1j_2}(b)$ is defined by*

$$\max_{\ell,q,\pi,s} \left\{ \begin{array}{rl} \max\limits_{w_1\in V(G_{j_1})} \left\{\pi_{w_1} - \pi_{w_1}^+\right\} + \max\limits_{w_2\in V(G_{j_2})} \left\{\pi_{w_2}^- - \pi_{w_2}\right\} & \\ - \sum\limits_{\substack{a\in P(G_{j_1},G_{j_2}):\\ a\in A_{\mathrm{cm}}^{j_1,\rightarrow}\cup A_{\mathrm{cv}}^{j_1,\leftarrow}}} \Delta_a^+ s_a & : (\mathrm{UL}) \end{array} \right\}.$$

We introduce variables θ_j^+ and θ_j^- for every $G_j\in\mathcal{G}$ that satisfy

$$\theta_j^+ = \max_{u\in V(G_j)} \left\{\pi_u - \pi_u^+\right\}, \tag{16a}$$

$$\theta_j^- = \max_{u\in V(G_j)} \left\{\pi_u^- - \pi_u\right\}. \tag{16b}$$

The optimal value function (15) then is a piecewise-linear function with $(|A_{\mathrm{act}}|+1)^2$ pieces. For $G_j\in\mathcal{G}$, θ_j^+ and θ_j^- are also piecewise-linear functions with each $|V(G_j)|$ pieces. The characterization in Corollary 6.5 requires optimizing $(|A_{\mathrm{act}}|+1)^2$ pieces of (15) separately, under the additional Constraint (16a) for $G_{j_1}\in\mathcal{G}$ and Constraint (16b) for $G_{j_2}\in\mathcal{G}$.

6.3 Separable optimal value function

Still considering the lower level as a problem defined on the reduced network $\tilde{G}$, we derive a third closed-form expression of the lower-level optimal value function φ. We can go one step further to reduce the number of subproblems in a characterization from $(|A_{\mathrm{act}}|+1)^2$ to $|A_{\mathrm{act}}|+1$. Instead of considering every pair of subnetworks

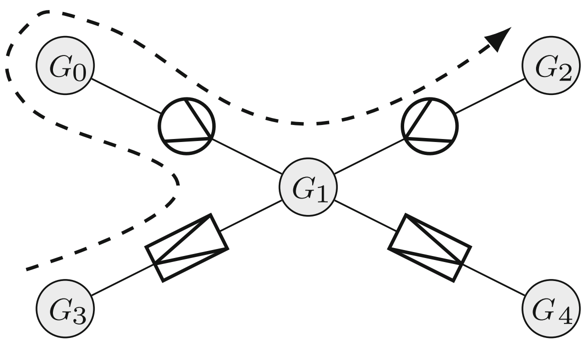

Fig. 3 Illustration of (17)

$(G_{j_1}, G_{j_2}) \in \mathcal{G}^2$ directly, the intuition is to first consider a third subnetwork G_k acting as an intermediary and then to treat (G_{j_1}, G_k) and (G_k, G_{j_2}) separately. Note that for any three subnetworks $G_{j_1}, G_k, G_{j_2} \in \mathcal{G}$, it holds that

$$
\begin{aligned}
&P(G_{j_1}, G_{j_2}) \cap \left(A_{\mathrm{cm}}^{j_1,\rightarrow} \cup A_{\mathrm{cv}}^{j_1,\leftarrow}\right) \\
&\quad \subseteq \left(P(G_k, G_{j_1}) \cap (A_{\mathrm{cm}}^{k,\leftarrow} \cup A_{\mathrm{cv}}^{k,\rightarrow})\right) \cup \left(P(G_k, G_{j_2}) \cap (A_{\mathrm{cm}}^{k,\rightarrow} \cup A_{\mathrm{cv}}^{k,\leftarrow})\right),
\end{aligned}
\tag{17}
$$

where equality holds if G_k lies on the path $P(G_{j_1}, G_{j_2})$. Figure 3 illustrates this relation for $G_{j_1} = G_3, G_k = G_0, G_{j_2} = G_2$. Here, the arc (G_0, G_1) appears in the right-hand side of (17), while clearly not lying on $P(G_3, G_2)$.

The previous observation allows us to prove the following result.

Lemma 6.6 *For every $G_k \in \mathcal{G}$, it holds $\varphi \geq \varphi^k$, where we define*

$$
\begin{aligned}
\varphi^k(\ell, q, \pi, s) := &\max_{\substack{G_{j_1} \in \mathcal{G}, \\ w_1 \in V(G_{j_1})}} \left\{ \pi_{w_1} - \pi_{w_1}^+ - \sum_{\substack{a \in P(G_k, G_{j_1}): \\ a \in A_{\mathrm{cm}}^{k,\leftarrow} \cup A_{\mathrm{cv}}^{k,\rightarrow}}} \Delta_a^+ s_a \right\} \\
&+ \max_{\substack{G_{j_2} \in \mathcal{G}, \\ w_2 \in V(G_{j_2})}} \left\{ \pi_{w_2}^- - \pi_{w_2} - \sum_{\substack{a \in P(G_k, G_{j_2}): \\ a \in A_{\mathrm{cm}}^{k,\rightarrow} \cup A_{\mathrm{cv}}^{k,\leftarrow}}} \Delta_a^+ s_a \right\}
\end{aligned}
\tag{18}
$$

for every feasible point (ℓ, q, π, s) of (UL).

Proof Given that $\Delta_a^+ s_a \geq 0$ for all $a \in A_{\mathrm{act}}$, (17) implies that $\varphi(\ell, q, \pi, s)$ is bounded from below by

$$
\max_{\substack{(G_{j_1}, G_{j_2}) \in \mathcal{G}^2, \\ w_1 \in V(G_{j_1}), \\ w_2 \in V(G_{j_2})}} \left\{ \pi_{w_1} - \pi_{w_1}^+ - \sum_{\substack{a \in P(G_k, G_{j_1}): \\ a \in A_{\mathrm{cm}}^{k,\leftarrow} \cup A_{\mathrm{cv}}^{k,\rightarrow}}} \Delta_a^+ s_a + \pi_{w_2}^- - \pi_{w_2} - \sum_{\substack{a \in P(G_k, G_{j_2}): \\ a \in A_{\mathrm{cm}}^{k,\rightarrow} \cup A_{\mathrm{cv}}^{k,\leftarrow}}} \Delta_a^+ s_a \right\}.
$$

For given G_k, the elements of the latter max-operator are separable w.r.t. (G_{j_1}, w_1) and (G_{j_2}, w_2). Consequently, the joint max-operator can be split, which concludes the proof. $\square$

Based on this result, we can derive the third closed form of the lower-level optimal value function φ by considering all $G_k \in \mathcal{G}$ and φ^k.

Theorem 6.7 *The optimal value function φ of (7) is given by*

$$\max_{G_k \in \mathcal{G}} \varphi^k, \tag{19}$$

where φ^k is defined in (18).

Proof By Lemma 6.6, $\varphi \geq \max_{G_k \in \mathcal{G}} \varphi^k$ holds. Let (ℓ, q, π, s) be feasible for (UL). Furthermore, let $(G_{j_1}, G_{j_2}, w_1, w_2)$ be the maximizer defining $\varphi(\ell, q, \pi, s)$. For G_k on the path $P(G_{j_1}, G_{j_2})$, equality holds in (17). Thus,

$$\max_{G_k \in \mathcal{G}} \varphi^k(\ell, q, \pi, s) = \varphi(\ell, q, \pi, s). \qquad \square$$

Again, we can solve several subproblems independently and obtain the third characterization.

Corollary 6.8 *Let $G = (V, A)$ be a weakly connected network satisfying Assumption 1. Then, the booking $b \in L$ is feasible if and only if $\phi_k(b) \leq 0$ is satisfied for a passive subnetwork $G_k \in \mathcal{G}$, where*

$$\phi_k(b) = \max_{\ell, q, \pi, s} \left\{ \varphi^k(\ell, q, \pi, s) \colon \text{(UL)} \right\}.$$

We introduce variables ϑ_k^+ and ϑ_k^- for every $G_k \in \mathcal{G}$ that satisfy

$$\vartheta_k^+ = \max_{\substack{G_j \in \mathcal{G}, \\ u \in V(G_j)}} \left\{ \pi_u - \pi_u^+ - \sum_{\substack{a \in P(G_k, G_j): \\ a \in A_{\mathrm{cm}}^{k,\leftarrow} \cup A_{\mathrm{cv}}^{k,\rightarrow}}} \Delta_a^+ s_a \right\}, \tag{20a}$$

$$\vartheta_k^- = \max_{\substack{G_j \in \mathcal{G}, \\ u \in V(G_j)}} \left\{ \pi_u^- - \pi_u - \sum_{\substack{a \in P(G_k, G_j): \\ a \in A_{\mathrm{cm}}^{k,\rightarrow} \cup A_{\mathrm{cv}}^{k,\leftarrow}}} \Delta_a^+ s_a \right\}. \tag{20b}$$

The optimal value function φ as defined in Theorem 6.7 then is a piecewise-linear function with $|A_{\mathrm{act}}| + 1$ pieces. For $G_k \in \mathcal{G}$, ϑ_k^+ and ϑ_k^- are also piecewise linear with $|V|$ pieces each. The characterization of Corollary 6.8 considers $|A_{\mathrm{act}}| + 1$ linear objectives. For each subproblem for $G_k \in \mathcal{G}$, only the additional constraints (20) corresponding to G_k are required.

As a closing remark, we discuss how the formulations and characterizations presented in this section can be implemented using standard linearization techniques for the max-operators.

Remark 6.9 (Linerization of max-operators) We have seen that the lower-level optimal value function is a piecewise-linear function that is convex and that needs to be maximized over a nonconvex domain. To model the max-operators involved in the different models of φ, we make use of the following classical technique. For a finite index set I, we want to model $\max_{i \in I}\{f_i\}$. To this end, we introduce binary variables u_i for all $i \in I$ and let $L, U \in \mathbb{R}$ be chosen such that $L \leq f_i \leq U$ holds for every $i \in I$. Then, $g = \max_{i \in I}\{f_i\}$ holds if and only if

$$f_i \leq g \leq f_i + (U - L)(1 - u_i), \quad i \in I, \tag{21a}$$

$$\sum_{i \in I} u_i = 1, \; u_i \in \{0, 1\}, \quad i \in I. \tag{21b}$$

This reformulation can be applied to all three variants (14), (15), and (19) of the lower-level optimal value function. The appropriate big-M values $L, U \in \mathbb{R}$ can be easily derived from the results of Sect. 5.2. By doing so, the three representations of the lower-level optimal value function φ (and the characterizations derived from them) can be modeled as MINLPs.

7 Computational experiments

In this section, we evaluate the performance of the different approaches developed in this paper. In Sect. 7.3, the presented nonlinear potential-based flow model is studied. In order to better evaluate the performance of our methods and to eliminate challenging nonlinearities, we additionally study a simplified linear potential-based flow model in Sect. 7.4. We compare the KKT reformulation with the three optimal-value-function reformulations and the three characterizations derived in Sect. 6. The columns Method and Definition of Table 1 give a short overview regarding the considered methods including their abbreviations used throughout this section.

7.1 Data

Our case study is based on two instances of the GasLib (Schmidt et al. 2017) and different corresponding bookings. On the one hand, we study GasLib-134 (version 2), which is a tree-shaped network with 134 nodes, one compressor, and one control valve. It roughly represents the Greek gas network. The flow thresholds m are set to 0 for the compressor and to -10^{-2} for the control valve. The latter value is chosen to guarantee the feasibility of the zero nomination in GasLib-134. Since the zero nomination is always booking-compliant, its feasibility is a necessary condition for the feasibility of any booking. Bookings for networks in the GasLib can be obtained by setting the corresponding nominations contained in the GasLib as bookings. For GasLib-134, these nominations reflect actual demand scenarios over several years in the past. We

Table 1 Overview of methods and model statistics

Method	Definition	GasLib-134		GasLib-40	
		Subproblems	Binaries	Subproblems	Binaries
KKT	(10)	1	272	1	90
F-OVF	(12) using (14)	1	17,956	1	1600
R-OVF	(12) using (15)	1	277	1	116
S-OVF	(12) using (19)	1	807	1	486
F-CHAR	Theorem 6.4	17,956	0	1600	0
R-CHAR	Corollary 6.5	9	162	36	44
S-CHAR	Corollary 6.8	3	268	6	80

selected three random nominations over the year to consider different demands. In particular, we study bookings derived from the nominations 2011-11-06, 2012-07-22, and 2014-10-24.

On the other hand, we consider the GasLib-40 network for which we have replaced one compressor by a pipe to satisfy Assumption 1. This results in a network with six fundamental cycles, 40 nodes, and five compressors. All flow thresholds m are set to 0. As before, we derive one booking, denoted by 0–0, from the single GasLib nomination. This booking then serves as a base for the generation of additional bookings. To do so, we slightly vary the booking at entries and exits as follows. For parameters $\mu_1, \mu_2 \in (0, 100)$ and node $u \in V$, we obtain a new booking $\tilde{b}$, denoted $\mu_1 - \mu_2$, by uniformly sampling a random integer in

$$\tilde{b}_u \in \begin{cases} \left[\frac{100-\mu_1}{100} b_u, \frac{100+\mu_1}{100} b_u\right], & \text{if } u \in V_+, \\ \left[\frac{100-\mu_2}{100} b_u, \frac{100+\mu_2}{100} b_u\right], & \text{if } u \in V_-, \\ \{0\}, & \text{if } u \in V_0, \end{cases}$$

where b is the initial booking 0–0. For GasLib-40, we generate three additional bookings for $(\mu_1, \mu_2) \in \{(10, 10), (1, 20), (10, 5)\}$. Note that in this way, we obtain bookings that are not balanced, which is in contrast to the bookings derived from GasLib nominations.

7.2 Computational setup

All models have been implemented in Python 3.8.0 using Pyomo 5.7.1 (Hart et al. 2017). We performed all computations using the Kaby Lake nodes with 32 GB RAM of the compute cluster Regionales Rechenzentrum Erlangen (2021). The time limit is 2 h.

In Sect. 7.3, when treating nonlinear gas physics, we use ANTIGONE 1.1 (Misener and Floudas 2014) and BARON 17.4 Tawarmalani and Sahinidis 2005) within GAMS 24.8 (GAMS Development Corporation 2020) to solve the occurring MINLPs.

We perform the computations on a single thread and set the optCr parameter in GAMS to 10^{-4}. In Sect. 7.4, we use Gurobi 9.0.1 (LLC Gurobi Optimization 2020) to solve linear approximations of the gas physics. We again perform computations on a single thread and set Gurobi parameters IntFeasTol to 10^{-9} and NumericFocus to 3.

We now discuss some statistics of our models, which are summarized in Table 1. To solve the single-level reformulations, a single optimization problem needs to be solved, whereas characterizations require solutions of multiple subproblems. The columns Subproblems present the number of optimization problems to be solved for each method w.r.t. the GasLib-134 and GasLib-40 networks. As we can see in Table 1, the number of subproblems drastically differs for the considered characterizations. This is due to the fact that F-CHAR consists of $|V|^2$ many subproblems, whereas the other two characterizations R-CHAR and S-CHAR consist of $(|A_{\text{act}}|+1)^2$ and $(|A_{\text{act}}|+1)$ subproblems. A reduced number of subproblems comes, however, at the cost of additional binary variables. All models are implemented in their linearized form, i.e., KKT's complementarity constraints have been linearized as discussed in Sect. 5.2 and for all other models, the linearization (21) of the max-operators is used. The Binaries columns indicate the maximum number of additional binary variables (other than the $|A_{\text{act}}|$ binary variables s) required for the linearization of a subproblem. Among all optimal-value-function reformulations, i.e., F-OVF, R-OVF, and S-OVF, we can observe that R-OVF contains the smallest number of binary variables, which is comparable to the number of binary variables for KKT. Regarding the characterizations, there is a clear trade-off between the number of subproblems and the number of binary variables, for which we later see that the large number of subproblems in F-CHAR is a computational disadvantage.

We finally note that all subproblems of the characterizations are solved iteratively without warm-starts. Thus, we do not exploit that all characterizations can be fully parallelized since all subproblems can be solved independently. The actual parallelization of the approaches based on the characterizations is out of the scope of this paper. However, to take this aspect into account during the discussion of our results, we discuss, besides the total sequential time, also an idealized parallel time, i.e., the maximum time required to solve a single subproblem.

7.3 The nonlinear case

Table 2 lists the results for the GasLib-134 network and the 2011-11-06 booking. Method indicates the method from Table 1. Vio. represents the obtained violation, i.e., for single-level reformulations the optimal value of the problem and for the characterizations the maximum violation of any bound on the optimal solutions of the corresponding subproblems. Thus, this column denotes the measure of feasibility of a booking. Positive values indicate violated potential bounds and thus the infeasibility of a booking. On the other hand, nonpositive values indicate that all booking-compliant nominations can be transported within the potential bounds, which implies the feasibility of a booking. Sol. gives the running time in seconds for single-level reformulations. Min., Med., and Max. denote the minimum, median, and maximum running times (in seconds) necessary for solving a single characterization subproblem and checking

Table 2 Results for GasLib-134 and the 2011-11-06 booking in the nonlinear case

Method	Solver	Vio.	Time				
			Sol.	Min.	Med.	Max.	Total
KKT	ANTIGONE	– 391.21	6.88				6.93
KKT	BARON	– 391.21	29.28				29.32
F-OVF	ANTIGONE	– 391.21	454.19				455.84
F-OVF	BARON	– 391.21	–				–
R-OVF	ANTIGONE	– 391.21	5.52				5.57
R-OVF	BARON	– 413.31	79.28				79.32
S-OVF	ANTIGONE	– 391.21	21.15				21.24
S-OVF	BARON	– 393.49	32.35				32.44
F-CHAR	ANTIGONE	– 391.21		0.22	0.28	3.17	6071.77
F-CHAR	BARON	– 391.21		0.23	0.30	3.71	6550.48
R-CHAR	ANTIGONE	– 391.21		0.30	1.04	20.24	53.44
R-CHAR	BARON	– 391.21		0.34	1.97	12.15	29.40
S-CHAR	ANTIGONE	– 391.21		0.92	2.40	231.93	235.35
S-CHAR	BARON	– 391.21		1.34	3.03	25.88	30.34

whether the corresponding bound on the optimal solution is satisfied. Finally, Total reports the total time, which for characterizations is equal to the time spent in the sequential treatment of all subproblems. If an instance could not be solved within the time limit of 2 h, then we represent it by "–" in the corresponding row of the table.

Unfortunately, the solvers do not give consistent results although all violations are negative, i.e., the booking seems to be feasible. The runs using BARON for R-OVF and S-OVF deviate from the common answer of all other combinations of methods and solvers. In particular, the optimal solution has been cut off from the search space at some point during the spatial branching. Consequently, we have to interpret the obtained results by BARON with great caution. On the other hand, we can analyze the trend presented by ANTIGONE. F-OVF and F-CHAR need the most time, which is expected since they have the most binary variables and subproblems, respectively. Although, the idealized parallel time of F-CHAR, i.e., 3.17s, is faster than the total time of KKT, it should not be forgotten that for GasLib-134, we need to solve 17,956 subproblems. Here, the only method slightly outperforming KKT is R-OVF. The latter has approximately the same number of additional binary variables as KKT, while S-OVF requires more binary variables. Concerning the corresponding methods using the characterizations, we observe that R-CHAR and S-CHAR are outperformed both w.r.t. the total sequential time and the idealized parallel time. Although, they require fewer subproblems to be solved than F-OVF, they admit additional binary variables to be branched on. For some subproblems, the solvers struggle to prove optimality. While the median time is good, there exist some outlier problems that require a long time to close the duality gap. As for the bookings 2012-07-22 and 2014-10-24, the general trends are similar although there are some outliers. KKT performs comparatively slow when considering the 2012-07-22 booking and using ANTIGONE. Similarly, S-OVF performs worse with ANTIGONE, whereas BARON follows the previous trend. For the sake of brevity, we include the tables corresponding to GasLib-134 and the 2012-07-22 and 2014-10-24 bookings in "Appendix A".

For GasLib-40, we are not able to generate meaningful results within the time limit of 2 h. We generally have to conclude that the problem at hand is numerically very unstable and hard to handle for the used nonlinear solvers. Some models could still be solved relatively fast, in particular the KKT model. However, the solvers often incorrectly certify optimality or get stuck in suboptimal solutions, not being able to close the duality gap. One possible explanation for this higher instability could be the cyclic structure of GasLib-40. To test this hypothesis, we generated variants of GasLib-134 with added cycles and compared them to the original tree network for the 2011-11-06 booking. We considered the GasLib-134 network with two, four, and six fundamental cycles added inside the passive subnetwork between both active elements. On the one hand, discrepancies between the results of ANTIGONE and BARON become more frequent with an increasing number of cycles. Furthermore, on the example of solving KKT using ANTIGONE, the running times for the GasLib-134 network with two, four, and six cycles are 42.64s, 871.41s, and 6553.46s, respectively. We thus observe a significant increase compared to the running time of 6.93s for the original GasLib-134 network.

The spatial branching on the nonlinear gas physics in addition to the branching on linearized piecewise-linear functions leads to very challenging problems, which would require further tuning of the MINLP solvers. This is, however, out of the scope of this case study. To compare our methods, we have thus resorted to analyzing linear approximations of gas physics as presented in the next section.

7.4 The linear case

Except for the nonlinear gas physics at the right-hand side of (1b), all considered models are linear with mixed-integer variables. In this section, we consider linear approximations of gas physics to obtain mixed-integer linear problems (MILP) to be solved by Gurobi. To this end, we replace $|q_a|$ for every $a \in A_{\text{pipe}}$ by cM, where $c \in (0, 1]$ is a scaling factor and $M := \min\{\sum_{u \in V_+} b_u, \sum_{u \in V_-} b_u\}$ is an upper bound on the flow on each arc. Thus, we replace Constraints (1b) with

$$\pi_u - \pi_v = \xi_a q_a, \quad \xi_a = c\Lambda_a M, \quad a = (u, v) \in A_{\text{pipe}}.$$

Table 3 shows the results for GasLib-134 and the 2011-11-06 booking, where Appr. indicates the different scaling factors $c \in \{0.2, 0.4, 0.6, 0.8, 1.0\}$. F-OVF is clearly outperformed by the shown methods. The same holds for F-CHAR both w.r.t. the total sequential time and the idealized parallel time. Consequently, we choose to omit both methods in the tables.

First, we observe that all methods present consistent results in the linear case. Additionally, for increasing scaling factors c, the resulting violations also increase. This trend is easily explained by the fact that a large scaling factor leads to a larger potential drop along all pipes, which again results in larger overall potential differences. In particular, the booking is feasible for $c \in \{0.2, 0.4\}$ and becomes infeasible

Table 3 Results for GasLib-134 and the 2011-11-06 booking in the linear case

Method	Appr.	Vio.	Time				
			Sol.	Min.	Med.	Max.	Total
KKT	0.2	– 377.15	2.71				2.75
R-OVF	0.2	– 377.15	2.02				2.06
S-OVF	0.2	– 377.15	4.53				4.62
R-CHAR	0.2	– 377.15		0.14	0.24	0.65	2.87
S-CHAR	0.2	– 377.15		0.64	1.13	1.14	3.00
KKT	0.4	– 174.10	3.03				3.07
R-OVF	0.4	– 174.10	2.87				2.92
S-OVF	0.4	– 174.10	6.77				6.87
R-CHAR	0.4	– 174.10		0.17	0.26	1.46	3.86
S-CHAR	0.4	– 174.10		0.85	0.97	1.15	3.06
KKT	0.6	384.11	3.47				3.51
R-OVF	0.6	384.11	1.26				1.31
S-OVF	0.6	384.11	9.92				10.01
R-CHAR	0.6	384.11		0.17	0.24	0.67	3.40
S-CHAR	0.6	384.11		0.77	0.90	1.00	2.76
KKT	0.8	966.75	3.24				3.29
R-OVF	0.8	966.75	2.81				2.86
S-OVF	0.8	966.75	10.30				10.39
R-CHAR	0.8	966.75		0.16	0.24	0.64	3.05
S-CHAR	0.8	966.75		0.80	0.82	1.11	2.81
KKT	1.0	1549.40	3.66				3.70
R-OVF	1.0	1549.40	2.70				2.74
S-OVF	1.0	1549.40	16.34				16.43
R-CHAR	1.0	1549.40		0.15	0.25	0.68	3.19
S-CHAR	1.0	1549.40		0.78	0.91	1.12	2.90

for larger scaling factors. We observe that for all scaling factors, KKT is performing well. Although slightly faster, R-OVF does not significantly outperform KKT. Similarly, S-OVF admits running times comparable to KKT, but is the slowest among the presented methods, which can be explained by its large number of binary variables necessary for the complete linearization of the optimal value function (19). Concerning the methods using the characterizations, the sequential time necessary to solve R-CHAR and S-CHAR is of the same order of magnitude as KKT. When considering the idealized parallel time, R-CHAR and S-CHAR are the clear winners. To obtain these idealized parallel times, 9 and 3 subproblems need to be solved in parallel, respectively. In that regard, R-CHAR is the fastest method for four scaling factors and only takes a little longer for $c = 0.4$, where S-CHAR is slightly faster. Again, similar trends can be observed for the remaining bookings of GasLib-134. We therefore do not explicitly discuss the corresponding results, but list them in "Appendix B".

Table 4 Results for GasLib-40 and the 0–0 booking in the linear case

Method	Appr.	Vio.	Time				
			Sol.	Min.	Med.	Max.	Total
KKT	0.2	1792.45	2.79				2.83
F-OVF	0.2	1792.45	15.24				15.45
R-OVF	0.2	1792.45	7.38				7.43
F-CHAR	0.2	1792.45		0.10	0.12	0.47	197.37
R-CHAR	0.2	1792.45		0.11	0.12	0.44	5.23
S-CHAR	0.2	1792.45		1.68	1.92	2.06	11.44
KKT	0.4	10247.01	2.75				2.80
F-OVF	0.4	10247.01	15.08				15.28
R-OVF	0.4	10247.01	16.33				16.38
F-CHAR	0.4	10247.01		0.10	0.13	0.47	204.01
R-CHAR	0.4	10247.01		0.12	0.13	0.46	5.67
S-CHAR	0.4	10247.01		1.72	1.95	2.58	12.54
KKT	0.6	18701.58	5.80				5.85
F-OVF	0.6	18701.58	15.99				16.18
R-OVF	0.6	18701.58	13.62				13.67
F-CHAR	0.6	18701.58		0.09	0.12	0.41	193.04
R-CHAR	0.6	18701.58		0.12	0.13	0.45	5.62
S-CHAR	0.6	18701.58		0.84	1.46	1.70	8.44
KKT	0.8	27156.15	2.92				2.97
F-OVF	0.8	27156.15	15.28				15.48
R-OVF	0.8	27156.15	8.18				8.23
F-CHAR	0.8	27156.15		0.10	0.12	1.13	195.71
R-CHAR	0.8	27156.15		0.11	0.13	0.44	5.50
S-CHAR	0.8	27156.15		1.24	1.76	2.00	10.00
KKT	1.0	35610.71	4.57				4.62
F-OVF	1.0	35610.71	15.77				15.96
R-OVF	1.0	35610.71	135.86				135.91
F-CHAR	1.0	35610.71		0.10	0.12	0.42	192.54
R-CHAR	1.0	35610.71		0.11	0.12	0.44	5.31
S-CHAR	1.0	35610.71		1.10	1.67	2.04	9.97

Table 4 shows the results for GasLib-40 and booking 0–0. In contrast to GasLib-134, F-OVF and F-CHAR are more competitive for GasLib-40, which has fewer nodes and thus both methods require fewer binary variables (for the linearizations) or subproblems; see Table 1. However, the cyclic structure of GasLib-40 makes the problem of checking the feasibility of a booking more challenging. In our experiments, S-OVF is not able to find a provably optimal solution and has thus been omitted from this table. For $c \in \{0.4, 0.6, 0.8, 1.0\}$, the optimal solution was found by S-OVF, however the duality gap could not be closed during the time limit. Overall, we observe more variability in running times across different scaling factors c for all methods. In terms of total time, i.e., the sequential time for characterizations, KKT is the fastest method. In terms of idealized parallel time, i.e., the maximum time necessary to solve a single subproblem, all three characterizations outperform KKT. Note that we still have to solve 1600 subproblems for F-CHAR, although all individual computations can be done in at most 0.5s for $c \in \{0.2, 0.4, 0.6, 1.0\}$ and in roughly 1s for $c = 0.8$. If computations can be fully parallelized, i.e., a sufficient number of cores are available to solve all subproblems in parallel, R-CHAR is the most adequate method for GasLib-40 to obtain a beneficial trade-off between the small number of subproblems to be solved and the number of additional binary variable in each subproblem. On the other hand, S-CHAR requires more time for each subproblem, at the benefit of very few subproblems to be solved and can thus still outperform KKT if fewer parallel computing resources are available.

To eliminate the possibility that the interpretation of the previous results are purely linked to the balancedness of bookings generated from nominations of the GasLib, we have additionally studied the three perturbed bookings 10–10, 1–20, and 10–5. Qualitatively, the results follow the discussion of the booking 0–0. The corresponding tables are thus listed in "Appendix C".

As a final discussion, note that all of the methods studied in this paper also allow for preemptive decisions without the need to solve the models to optimality. For each single-level reformulation, whenever a relaxation produces a nonpositive value, we can stop the computation and certify that the booking is feasible. Similarly, whenever a feasible point of positive violation is found, the booking is infeasible with the certificate given by the corresponding infeasible nomination. For showing the infeasibility of a booking, the same logic can be extended to characterizations. As soon as a feasible point of one subproblem with positive violation has been found, we can stop and certify that the booking is infeasible. This can be useful especially in practice, since TSOs generally have additional knowledge regarding their networks and are aware of their bottlenecks. With this knowledge at hand, it could be possible to check specific individual subproblems to identify infeasible nominations that lead to a rejection of the considered booking request. In case of a feasible booking, all subproblems must be solved. They can however be terminated early, based on a nonpositive value of a relaxation.

8 Conclusion

The problem of deciding the feasibility of a booking in the European entry-exit gas market has been studied mostly for passive networks up to now. In this paper, we considered networks with linearly modeled active elements that do not lie on cycles of the network. By doing so, we present a first stepping stone towards the study of more general networks and more general models of active elements. The approaches for verifying the feasibility of a booking in passive networks are not directly applicable to the case of networks with active elements, as discussed in Sect. 3. Thus, we have then presented a bilevel optimization model, in which the upper-level player chooses a nomination that is most difficult to transport and the TSO at the lower level uses the active elements to transport this nomination. Consequently, the bilevel structure results from the fact that the TSO takes a decision individually for every nomination by controlling the active elements appropriately. We studied both the classical KKT reformulation and problem-specific optimal-value-function reformulations. More precisely, we have given three optimal-value-function reformulations giving rise to three equivalent characterizations of feasible bookings, which generalize the characterization in Labbé et al. (2020) for passive networks. Our case studies show that the KKT approach is already a very well performing method to check the feasibility of a booking. It also shows that the more problem-specific approaches of Sect. 6 can sometimes outperform the KKT approach, especially when parallel computing resources are available. It should, however, be noted that the applicability of these methods depends on the structure of the network at hand. In particular, the number of binary variables for the linearizations and the number of subproblems to be solved in the characterizations vary significantly. They are determined by the number of active elements and nodes. Thus, the best-performing method among the various optimal-value-function reformulations and characterizations strongly depends on the considered network.

In general, the methods developed in this paper can be used as a decision-support system in the planning departments of TSOs that decide on the signing or the rejection of booking requests. In practice, the validation of such a booking request is usually based on checking expert scenarios via simulation tools. In this regard, our methods can help to automatically generate such expert scenarios that are hard to transport within the technical restrictions of the network. Obviously, this is only possible if the network satisfies the assumptions made in this paper and, thus, there is still a lot to do in order to automate the process of validating bookings.

For future work, it will be interesting to study networks without specific assumptions on the location of the active elements, as well as more general models for the active elements. However, even in the setting of this paper, some challenges still need to be tackled. It is required to develop problem-specific solution approaches, especially for the case of nonlinear gas physics. Similar to the studies in Robinius et al. (2019); Labbé et al. (2020) for tree-shaped and in Labbé et al. (2021) for single-cycle networks, algorithms to solve the nonlinear subproblems of the characterizations presented in this paper can be beneficial. Finally, the analyses of the European gas market models studied in Böttger et al. (2021); Schewe et al. (2020) can be extended to take into account linearly modeled active elements by integrating the novel characterizations of feasible bookings presented in this paper.

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Appendix A: Results for the nonlinear case

See Tables 5 and 6.

Table 5 Results for GasLib-134 and the 2012-07-22 booking

Method	Solver	Vio.	Time				
			Sol.	Min.	Med.	Max.	Total
KKT	ANTIGONE	– 514.36	420.38				420.43
KKT	BARON	– 514.36	47.93				47.97
F-OVF	ANTIGONE	– 514.36	–				–
F-OVF	BARON	– 514.36	–				–
R-OVF	ANTIGONE	– 514.36	192.06				192.11
R-OVF	BARON	– 514.36	38.82				38.86
S-OVF	ANTIGONE	– 514.36	1873.64				1873.73
S-OVF	BARON	– 514.36	67.75				67.84
F-CHAR	ANTIGONE	– 514.36		0.21	0.27	6.23	5942.30
F-CHAR	BARON	– 514.36		0.19	0.31	181.02	10490.60
R-CHAR	ANTIGONE	– 514.36		0.25	0.82	24.72	67.74
R-CHAR	BARON	– 514.36		0.34	0.93	8.83	19.48
S-CHAR	ANTIGONE	– 514.36		0.62	188.47	222.48	411.66
S-CHAR	BARON	– 514.36		1.13	18.23	43.84	63.28

Table 6 Results for GasLib-134 and the 2014-10-24 booking

Method	Solver	Vio.	Time				
			Sol.	Min.	Med.	Max.	Total
KKT	ANTIGONE	– 512.80	4.41				4.45
KKT	BARON	– 512.80	6.13				6.18
F-OVF	ANTIGONE	– 512.80	–				–
F-OVF	BARON	– 512.80	–				–
R-OVF	ANTIGONE	– 512.80	2.27				2.32
R-OVF	BARON	– 512.80	8.75				8.79
S-OVF	ANTIGONE	– 512.80	4.28				4.37
S-OVF	BARON	– 512.80	42.08				42.17
F-CHAR	ANTIGONE	– 512.80		0.22	0.27	1.45	5065.65
F-CHAR	BARON	– 512.80		0.19	0.27	19.05	5069.69
R-CHAR	ANTIGONE	– 512.80		0.24	0.52	24.00	46.63
R-CHAR	BARON	– 512.80		0.33	0.79	3.10	10.71
S-CHAR	ANTIGONE	– 512.80		0.42	1.78	71.49	73.78
S-CHAR	BARON	– 512.80		0.83	3.12	21.97	26.00

Appendix B: Results for GasLib-134 in the linear case

See Tables 7 and 8.

Table 7 Results for GasLib-134 and the 2012-07-22 booking

Method	Appr.	Vio.	Time				
			Sol.	Min.	Med.	Max.	Total
KKT	0.2	– 512.56	1.72				1.76
R-OVF	0.2	– 512.56	1.22				1.27
S-OVF	0.2	– 512.56	4.47				4.56
R-CHAR	0.2	– 512.56		0.15	0.24	0.76	3.25
S-CHAR	0.2	– 512.56		0.78	0.80	0.96	2.63
KKT	0.4	– 500.12	2.48				2.52
R-OVF	0.4	– 500.12	1.65				1.70
S-OVF	0.4	– 500.12	5.11				5.20
R-CHAR	0.4	– 500.12		0.17	0.26	0.83	3.35
S-CHAR	0.4	– 500.12		0.86	0.92	1.07	2.94
KKT	0.6	– 276.34	3.24				3.29
R-OVF	0.6	– 276.34	2.17				2.21
S-OVF	0.6	– 276.34	6.48				6.57
R-CHAR	0.6	– 276.34		0.15	0.25	0.60	3.21
S-CHAR	0.6	– 276.34		0.64	0.82	1.06	2.60
KKT	0.8	86.17	3.13				3.17
R-OVF	0.8	86.17	2.29				2.34
S-OVF	0.8	86.17	15.61				15.70
R-CHAR	0.8	86.17		0.17	0.26	1.23	3.72
S-CHAR	0.8	86.17		0.68	0.89	1.04	2.70
KKT	1.0	448.67	3.15				3.20
R-OVF	1.0	448.67	2.62				2.66
S-OVF	1.0	448.67	11.46				11.55
R-CHAR	1.0	448.67		0.14	0.27	0.62	3.01
S-CHAR	1.0	448.67		0.71	0.81	1.08	2.69

Table 8 Results for GasLib-134 and the 2014-10-24 booking

Method	Appr.	Vio.	Time				
			Sol.	Min.	Med.	Max.	Total
KKT	0.2	– 513.71	2.04				2.08
R-OVF	0.2	– 513.71	1.03				1.08
S-OVF	0.2	– 513.71	3.11				3.20
R-CHAR	0.2	– 513.71		0.15	0.23	0.49	2.33
S-CHAR	0.2	– 513.71		0.38	0.41	0.74	1.62
KKT	0.4	– 502.41	1.89				1.94
R-OVF	0.4	– 502.41	1.31				1.35
S-OVF	0.4	– 502.41	2.82				2.91
R-CHAR	0.4	– 502.41		0.15	0.22	0.55	2.53
S-CHAR	0.4	– 502.41		0.40	0.57	0.74	1.81
KKT	0.6	– 491.12	1.94				1.99
R-OVF	0.6	– 491.12	1.09				1.13
S-OVF	0.6	– 491.12	3.41				3.51
R-CHAR	0.6	– 491.12		0.15	0.23	0.54	2.49
S-CHAR	0.6	– 491.12		0.40	0.53	0.76	1.79
KKT	0.8	– 479.82	2.14				2.18
R-OVF	0.8	– 479.82	1.19				1.23
S-OVF	0.8	– 479.82	3.84				3.93
R-CHAR	0.8	– 479.82		0.15	0.23	0.72	2.80
S-CHAR	0.8	– 479.82		0.43	0.50	0.83	1.85
KKT	1.0	– 468.53	2.31				2.36
R-OVF	1.0	– 468.53	1.16				1.20
S-OVF	1.0	– 468.53	4.08				4.17
R-CHAR	1.0	– 468.53		0.15	0.24	0.67	2.78
S-CHAR	1.0	– 468.53		0.43	0.62	0.81	1.95

Appendix C: Results for GasLib-40 in the linear case

See Table 9, 10 and 11.

Table 9 Results for GasLib-40 and the 10–10 booking

Method	Appr.	Vio.	Time				
			Sol.	Min.	Med.	Max.	Total
KKT	0.2	1444.25	2.69				2.74
F-OVF	0.2	1444.25	13.93				14.13
R-OVF	0.2	1444.25	35.23				35.28
F-CHAR	0.2	1444.25		0.10	0.13	0.42	204.48
R-CHAR	0.2	1444.25		0.12	0.14	0.55	5.88
S-CHAR	0.2	1444.25		0.79	1.76	2.41	9.74
KKT	0.4	9550.63	3.30				3.35
F-OVF	0.4	9550.63	15.21				15.40
R-OVF	0.4	9550.63	12.47				12.52
F-CHAR	0.4	9550.63		0.10	0.12	0.46	194.77
R-CHAR	0.4	9550.63		0.12	0.14	0.52	6.33
S-CHAR	0.4	9550.63		0.79	1.86	2.04	9.43
KKT	0.6	17657.00	2.99				3.04
F-OVF	0.6	17657.00	16.23				16.43
R-OVF	0.6	17657.00	21.40				21.45
F-CHAR	0.6	17657.00		0.10	0.12	0.43	192.77
R-CHAR	0.6	17657.00		0.11	0.14	0.43	5.58
S-CHAR	0.6	17657.00		0.80	1.67	1.92	9.45
KKT	0.8	25763.37	4.07				4.11
F-OVF	0.8	25763.37	18.91				19.10
R-OVF	0.8	25763.37	44.41				44.46
F-CHAR	0.8	25763.37		0.09	0.12	0.47	196.67
R-CHAR	0.8	25763.37		0.12	0.14	0.43	5.61
S-CHAR	0.8	25763.37		1.10	1.71	2.05	9.71
KKT	1.0	33869.75	3.56				3.61
F-OVF	1.0	33869.75	17.81				18.00
R-OVF	1.0	33869.75	189.46				189.51
F-CHAR	1.0	33869.75		0.11	0.13	0.57	208.23
R-CHAR	1.0	33869.75		0.12	0.13	0.44	5.64
S-CHAR	1.0	33869.75		1.72	1.83	2.12	11.23

Table 10 Results for GasLib-40 and the 1–20 booking

Method	Appr.	Vio.	Time				
			Sol.	Min.	Med.	Max.	Total
KKT	0.2	1859.32	3.14				3.19
F-OVF	0.2	1859.32	13.59				13.79
R-OVF	0.2	1859.32	86.28				86.34
F-CHAR	0.2	1859.32		0.10	0.13	0.51	206.26
R-CHAR	0.2	1859.32		0.11	0.14	0.46	5.78
S-CHAR	0.2	1859.32		1.60	1.97	2.52	11.89
KKT	0.4	10380.76	3.79				3.84
F-OVF	0.4	10380.76	15.04				15.24
R-OVF	0.4	10380.76	27.46				27.52
F-CHAR	0.4	10380.76		0.10	0.13	0.45	204.29
R-CHAR	0.4	10380.76		0.12	0.14	0.43	5.74
S-CHAR	0.4	10380.76		1.53	1.99	2.68	12.65
KKT	0.6	18902.19	4.79				4.84
F-OVF	0.6	18902.19	15.04				15.24
R-OVF	0.6	18902.19	20.71				20.76
F-CHAR	0.6	18902.19		0.10	0.13	0.53	201.68
R-CHAR	0.6	18902.19		0.11	0.14	0.43	5.84
S-CHAR	0.6	18902.19		0.82	1.78	2.18	9.92
KKT	0.8	27423.63	2.98				3.02
F-OVF	0.8	27423.63	15.73				15.92
R-OVF	0.8	27423.63	10.80				10.85
F-CHAR	0.8	27423.63		0.10	0.13	0.44	203.74
R-CHAR	0.8	27423.63		0.11	0.13	0.45	5.65
S-CHAR	0.8	27423.63		0.86	1.82	2.09	9.42
KKT	1.0	35945.07	2.26				2.31
F-OVF	1.0	35945.07	19.88				20.08
R-OVF	1.0	35945.07	44.83				44.88
F-CHAR	1.0	35945.07		0.10	0.13	0.52	205.41
R-CHAR	1.0	35945.07		0.11	0.13	0.45	5.64
S-CHAR	1.0	35945.07		0.84	1.74	2.03	9.64

Table 11 Results for GasLib-40 and the 10–5 booking

Method	Appr.	Vio.	Time				
			Sol.	Min.	Med.	Max.	Total
KKT	0.2	1575.16	6.37				6.42
F-OVF	0.2	1575.16	14.09				14.29
R-OVF	0.2	1575.16	55.73				55.78
F-CHAR	0.2	1575.16		0.10	0.12	0.42	203.09
R-CHAR	0.2	1575.16		0.12	0.13	0.52	5.71
S-CHAR	0.2	1575.16		1.71	2.07	2.43	12.38
KKT	0.4	9812.44	2.60				2.65
F-OVF	0.4	9812.44	17.19				17.38
R-OVF	0.4	9812.44	30.15				30.20
F-CHAR	0.4	9812.44		0.10	0.12	0.42	199.62
R-CHAR	0.4	9812.44		0.12	0.13	0.49	5.61
S-CHAR	0.4	9812.44		1.25	2.06	2.76	11.86
KKT	0.6	18049.72	2.45				2.50
F-OVF	0.6	18049.72	14.59				14.79
R-OVF	0.6	18049.72	68.87				68.92
F-CHAR	0.6	18049.72		0.10	0.13	0.45	203.72
R-CHAR	0.6	18049.72		0.12	0.13	0.51	5.70
S-CHAR	0.6	18049.72		1.19	1.65	1.91	9.56
KKT	0.8	26287.00	2.79				2.84
F-OVF	0.8	26287.00	16.32				16.52
R-OVF	0.8	26287.00	72.69				72.74
F-CHAR	0.8	26287.00		0.10	0.13	0.55	208.26
R-CHAR	0.8	26287.00		0.11	0.13	0.52	5.66
S-CHAR	0.8	26287.00		0.83	1.14	2.13	8.08
KKT	1.0	34524.28	3.06				3.11
F-OVF	1.0	34524.28	16.32				16.52
R-OVF	1.0	34524.28	40.98				41.03
F-CHAR	1.0	34524.28		0.10	0.12	0.52	196.73
R-CHAR	1.0	34524.28		0.11	0.14	0.49	5.92
S-CHAR	1.0	34524.28		0.88	1.73	1.99	9.39

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Article 6

Modeling hydrogen networks for future energy systems: A comparison of linear and nonlinear approaches

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Modeling Hydrogen Networks for Future Energy Systems: A Comparison of Linear and Nonlinear Approaches

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Abstract

Common energy system models that integrate hydrogen transport in pipelines typically simplify fluid flow models and reduce the network size in order to achieve solutions quickly. This contribution analyzes two different types of pipeline network topologies (namely, star and tree networks) and two different fluid flow models (linear and nonlinear) for a given hydrogen capacity scenario of electrical reconversion in Germany to analyze the impact of these simplifications. For each network topology, robust demand and supply scenarios are generated. The results show that a simplified topology, as well as the consideration of detailed fluid flow, could heavily influence the total pipeline investment costs. For the given capacity scenario, an overall cost reduction of the pipeline costs of 37% is observed for the star network with linear cost compared to the tree network with nonlinear fluid flow. The impact of these improvements regarding the total electricity reconversion costs has led to a cost reduction of 1.4%, which is fairly small. Therefore, the integration of nonlinearities into energy system optimization models is not recommended due to their high computational burden. However, the applied method for generating robust demand and supply scenarios improved the credibility and robustness of the network topology, while the simplified fluid flow consideration can lead to infeasibilities. Thus, we suggest the utilization of the nonlinear model for post-processing to prove the feasibility of the results and strengthen their credibility, while retaining the computational performance of linear modeling.

Keywords

Hydrogen reconversion; Hydrogen infrastructure; Spatial resolution; Pipeline design optimization; Pressure drop; Robust optimization

1. Introduction

The mitigation of greenhouse gas emissions to tackle climate change is one of the main challenges facing upcoming generations [1]. It is broadly accepted that high shares of renewable energies such as photovoltaic or wind power systems are necessary to replace fossil energy carriers [2]. However, the weather dependencies of renewables necessitate the implementation of large-scale storage systems. Hydrogen represents a chemical storage technology with high energy density and long-term stability. Thus, the production of hydrogen enables the transfer of renewable energy into other sectors like transport [3] or heat [4], which may otherwise struggle to reach their greenhouse gas reduction targets.

Several studies deal with the integration of hydrogen into the future energy system. Yang and Ogden [5], for instance, investigate hydrogen transport and determine that transport through pipelines offers the lowest transmission costs for demand-intensive scenarios. Johnson and Ogden [6] show a spatially resolved hydrogen planning tool for long-term pipeline planning. Baufumé et al. [7], in turn, design a nationwide hydrogen pipeline grid for supplying 75% of the German transport sector and demonstrate the economic feasibility of hydrogen pipelines. André et al. [8] present an algorithm for the design of an hydrogen transmission pipeline network for the nationwide supply of future fuel cell vehicles in France. Reuß et al. [9], meanwhile, elaborate on different infrastructure technologies and show that the transmission of hydrogen via pipelines and its storage in underground formations like salt caverns are key technologies for future infrastructure development.

While these studies focus on hydrogen itself, the impact of integrating hydrogen in an energy system requires the presence of competitive technologies as well. Hence, the scientific community has developed various optimization models to evaluate the impact of hydrogen on the system as a whole. Welder et al. [10], for example, investigate a German hydrogen infrastructure with a spatio-temporal approach that focuses on the role of caverns for the infrastructure. In addition, the authors analyze an electrical reconversion scenario for the supply of North Rhine Westphalia and illustrate the important existence of hydrogen even with competing electricity transport [11]. Samsatli et al. [12, 13] investigate the UK energy system's capacity to supply hydrogen to the domestic transport or heat sectors. Moreno-Benito et al. [14], in turn, consider different hydrogen production options for evaluating cost-optimal hydrogen infrastructure development in the UK through 2100, neglecting a temporal resolution. Almansoori and Betancourt-Torcat [15], as well as Ochoa Bique and Zondervan [16], compute a nationwide hydrogen supply chain for Germany, in which they do not take hydrogen pipelines and temporal resolution into account. Weber and Papageorgiou [17], meanwhile, minimize network costs with consideration of hydraulics in hydrogen pipelines. However, the authors do not consider a temporal resolution to address the fluctuations of demand and supply.

The more sectors a techno-economic energy system model considers, the lower the degree of detail is typically allowed for the representation of infrastructure. This is caused by limitations of model size and computational tractability. Welder et al. [10, 11] therefore consider pipelines for hydrogen transport but neglect the effects of pressure drops by applying a fixed gas velocity and a linearization of pipeline costs for varying hydrogen flows. Samsatli et al. [12] consider just one pipeline diameter and define the maximum flowrate during preprocessing without taking different diameters into account. Similarly, Moreno-Benito et al. [14] allow the selection of six discrete diameters with a predefined maximum flowrate but without taking the pressure drops into account. In addition, Welder et al. [10, 11], Samsatli et al. [12], and Moreno-Benito and Agnolucci [14] create regions for the spatial resolution and utilize distance matrices for the estimation of transport distances from region to region.

Groissböck [18] reviewed 33 open source energy system optimization models and showed that not a single open source model considers physical constraints like pressure as part of the optimization. So far, the consideration of physical constraints for the gaseous flow in system design and network expansion was only implemented for stand-alone pipeline network models without optimizing the supply system at the same time. This is mainly due to computational performance losses resulting from the nonlinear pressure drop behavior of pipeline sizing as well as the increasing problem size with higher numbers of nodes. The impact of neglecting physical constraints of compressible fluid transport in techno-economic energy system models was not investigated so far.

Robinius et al. [19] thus present a novel approach to integrate the nonlinear pressure drop into a mixed-integer nonlinear pipeline design optimization model for tree-structured transport networks. To integrate the physical behavior of hydrogen, the authors further develop an approach used for operational optimization of the today's natural gas grid as used in Schmidt et al. [20, 21], see also Aßmann et al. [22]. To address fluctuating demand and production uncertainties, Robinius et al. [19] develop an algorithm for modeling "robust" demand scenarios. Optimizing with respect to these scenarios guarantees the feasibility of all balanced demands and supplies within previously given flow rates of sources, sinks, and storage options. Aside from these flow rates, the algorithm requires a predefined pipeline topology and the allocation of hydrogen sources, sinks, and storage options. The method is linked to the field of robust optimization, which aims at protecting an optimization problem from deterministic data uncertainties; see Gorissen et al. [23] for an introduction to robust optimization. In summary, the method is not suitable for optimizing the entire energy system. However, the robust demand and supply scenarios obtained allow for consideration of pressure drops in the entire network.

Samsatli et al. [12] and Moreno-Benito et al. [14] consider pressure losses during preprocessing to elaborate the maximum flowrate of each pipeline section. In theory, they require an additional compressor at each node to recompress the hydrogen to the maximum pressure level. With the nonlinear model of Robinius et al. [19], the pressure level in each pipe section is considered and made part of the optimization. As a result, the pipeline network is designed for avoiding compressor stations for recompression in the entire network.

In addition, spatially resolved energy system models typically use a regionalization with a simplification of transport options for "region-to-region" energy transport [10, 12, 14, 15, 17]. This assumption highly simplifies the pipeline network topology, especially for low numbers of regions. In contrast, pipeline design models that have a high spatial resolution like those of Baufumé et al. [7] or André et al. [24] compute the pipeline design without taking the costs of production and storage into account. The error arising from simplifying the pipeline network design and, respectively, the topology, has not yet been investigated.

With this contribution, we evaluate the effects of simplifications made in techno-economic energy system models regarding physical constraints and spatial resolution. These energy systems with integrated design of production, storage, and transport capacities simplify the transport of compressible fluids by simplifying network topologies and the considered fluid flow model at the same time. The focus of this work is to evaluate the impact of nonlinear pressure drop considerations, as well as the impact of topology design on hydrogen pipeline system feasibility and costs. To this end, we apply the model from Robinius et al. [19], which is briefly described in Subsection 2.1, to the pipeline topology and capacity scenario from Welder et al. [11] for two different network topologies, which are given in Subsection 2.2. In Section 3, the results regarding pipeline sizing, total system costs, differences between topologies, and flow modeling approaches are analyzed and discussed. Finally, the feasibility of the linear model is checked by a nonlinear model.

2. Methods and Data

This section introduces the methods used, as well as the data. In Figure 1, the two workflows for determining the pipeline topologies (Workflow I) and the resulting pipeline designs (Workflow II) for two different design methods are shown. Workflow I starts with a candidate pipeline grid that represents existing pipeline routes used for natural gas connected to the source, sink, and storage nodes of the demand and supply scenario. The geo-referenced pipeline data is taken from Welder et al. [11]. The candidate pipeline grid is then reduced to represent potential routes that could be selected during the optimization. Dijkstra's algorithm [25] is then used for creating shortest-path connections between source, sink, and storage nodes. The remaining grid represents the "tree network". To create the "star network", the real course of the pipes is neglected and, instead, centroid-to-centroid connections with one distance value for each connection are employed.

In Workflow II, the "capacity scenario" is first evaluated by performing an energy system optimization based on techno-economic input data and geo-referenced residual electricity loads. The capacity scenario consists of hydrogen injection and withdrawal time series and is taken from Welder et al. [11]. These time series are necessary for generating a robust scenario set according to the scenario generation algorithm of Robinius et al. [19]. As a result, demand and supply scenarios are generated for each pipeline topology, namely for the star network and tree network. Finally, two different approaches for modeling physical flow properties are applied. The linear model (LP) fixes the gas velocity and neglects the pressure as the driving force of fluid flow. The mixed-integer nonlinear model (MINLP), in turn, minimizes the total pipeline costs with respect to pressure drop in the pipes by using the discrete arc sizing optimization from Robinius et al. [19].

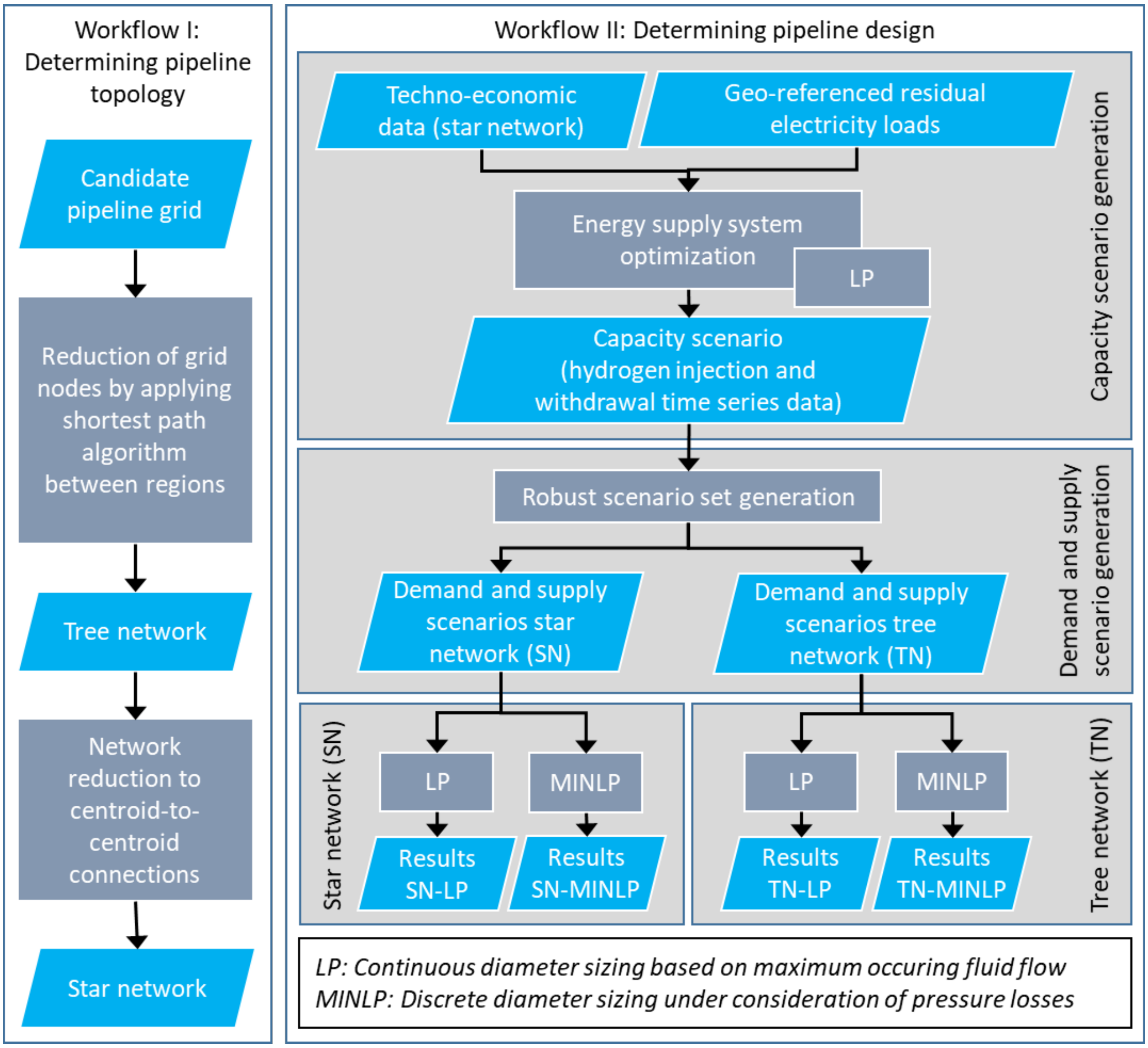

Figure 1. Explanation of the scenario and the workflows used in this study.

2.1 Pipeline Design Modeling

The modeling of the pipeline design uses either a linear or nonlinear fluid flow representation and aims to minimize the total pipeline costs.

The nonlinear model used in this study for minimizing the pipeline costs is developed and explained in detail in Robinius et al. [19]. The pressure drop is considered by using the Weymouth equation [20, 21, 26-28] for the approximated relationship between mass flow, diameter, and gas pressures. As the pipeline investment costs are mainly dependent on the pipeline diameters, the overall system costs are optimized by selecting the diameters. The model is set up with Pyomo [29, 30] and Gurobi [31] is used as the mixed-integer linear programming solver.

Aside from the medium (hydrogen), the main inputs for the model are the lower and upper pressure bounds and the discrete pipeline diameters. All pipelines are considered to operate between 70 and 100 bar. Pipeline diameters beyond DN1400 are not considered, as the application of looped pipes is more reasonable for such diameters. As the model can become infeasible without options for higher hydrogen flows, the method of Lenz and Schwarz [32] is used to calculate the equivalent pipeline diameter D for two looped pipes D_1 and D_2:

$$D = \left(D_1^{\frac{5}{2}} + D_2^{\frac{5}{2}} \right)^{\frac{2}{5}}. \tag{1}$$

The investment costs for the discrete diameters of the pipeline are considered according to an empirical cost analysis for natural gas pipelines designed for a pressure level of 100 bar from Mischner et al. [33]. The specific pipeline investment costs are dependent on the pipeline's diameter D in mm. As Mischner et al. [33] give pipeline costs for natural gas pipelines, their utilization with hydrogen is conservatively estimated to have 5% higher costs, similar to Welder et al. [11],

$$Invest = 1.05 \cdot 278.24 \cdot e^{1.6 \cdot D}, \tag{2}$$

with pipeline diameter D in m and specific investment costs in EUR/m.

The considered pipeline diameters and resulting specific investment costs are given in Table 1. The specific pipeline costs of Mischner are given in EUR with reference year 2011.

Table 1. Considered pipeline diameters and respective investment costs.

Name	Diameter (mm)	Investment costs (EUR/m)	Name	Diameter (mm)	Investment costs (EUR/m)
DN100	106	346	**DN750**	769	999
DN125	131	360	**DN800**	814	1,075
DN150	159	377	**DN850**	864	1,164
DN200	207	407	**DN900**	915	1,263
DN250	259	442	**DN950**	960	1,357
DN300	306	477	**DN1000**	1,011	1,473
DN325	336	500	**DN1050**	1,058	1,588
DN350	384	540	**DN1100**	1,104	1,709
DN400	432	583	**DN1150**	1,155	1,854
DN450	480	629	**DN1200**	1,249	2,155
DN500	527	679	**DN1300**	1,342	2,501
DN550	578	737	**DN1400**	1,444	2,944
DN600	625	794	**2xDN1200**	1,648	4,311
DN650	671	855	**2xDN1300**	1,771	5,002
DN700	722	927	**2xDN1400**	1,905	5,889

According to Samsatli et al. [34], the gas velocity inside pipelines is not only limited by pressure drop, but also by mechanical interferences. Excessively high gas velocities could lead to erosional behavior or high noise emissions. Therefore, the gas velocity must be limited. Although the pressure drop consideration itself leads to a limited possible gas velocity, an upper bound for the gas velocity is not implemented in the model of Robinius et al. [19]. Therefore, we added a constraint to the model that the velocity v in each pipeline must be less than or equal to compared to the predefined maximum gas velocity v_{max}.

For the linear case, the occurrence of a pressure drop inside the pipeline is neglected and a constant gas velocity is assumed, as in Welder et al. [11]. The corresponding pipeline costs are based on Equation (2). Welder et al. [11] linearize the pipeline investment after fixing the gas velocity inside the pipeline to 10 m/s and assume a fixed gas density of 5.7 kg_{H2}/m^3, similar to other studies [7, 10, 14], to keep the overall optimization problem solvable through a mixed-integer linear programming solver. The pipeline capacity is linked to the hydrogen flow by using the lower heating value of hydrogen of 33.32 kWh/kg_{H2}, where 1 GW_{H2} consequently corresponds to 8.34 kg_{H2}/s,

$$Invest_{linear} = 180 \cdot P + 408, \quad (3)$$

with a pipeline capacity P in GW_{H2} and specific pipeline investment $Invest_{linear}$ in (EUR/m).

On the left-hand side of Figure 2, the original cost function of Mischner et al. [33] for varying diameters is given. On the right-hand side of Figure 2, the linear approximated cost function of Equation (3) is compared to the basic costs function of Equation (2). While the linearization for low hydrogen flows slightly overestimates the investment costs, the general behavior is represented quite well. However, the velocity is fixed for that purpose, which is not the case for models considering a pressure drop.

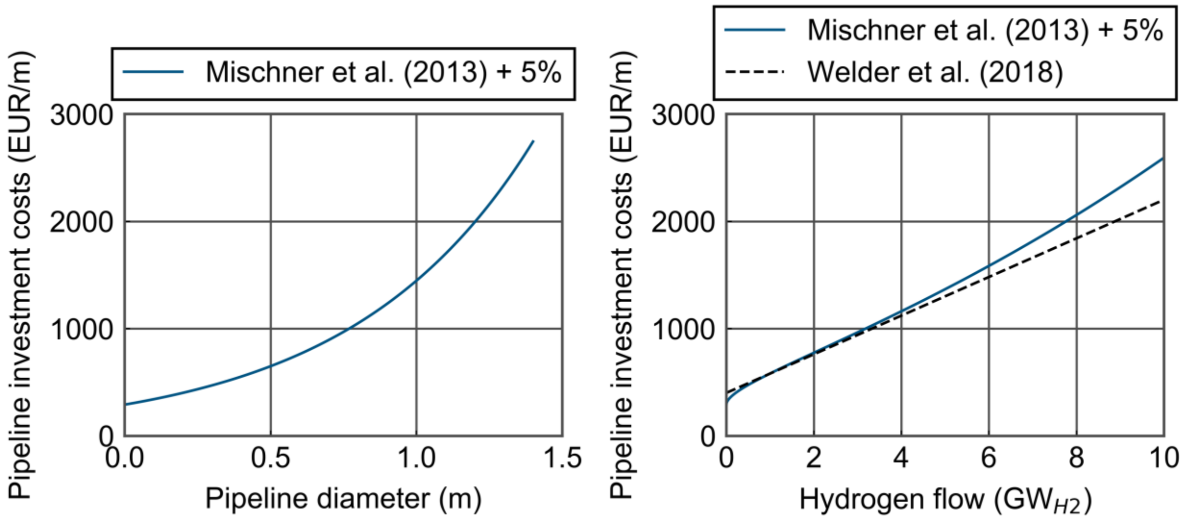

Figure 2. Left: pipeline investment costs dependent on pipeline diameter according to Mischner et al. [33]; right: adjusted pipeline investment costs from Mischner et al. [33], Equation (2), for gas velocity (10 m/s) and density (5.7 kg_{H2}/m^3) compared to the linearized cost function from Welder et al. [11], Equation (3), depending on the maximum flow.

To calculate the pipeline-specific expenditures as part of the levelized costs of electricity, a depreciation period for the pipeline of 40 years as well as a yearly operation and maintenance of 5 EUR per meter and year is assumed. The weighted average cost of capital (WACC) is set to 8% and annualized by calculating the annuity factor AF,

$$AF = \frac{(1+WACC)^{depreciation\ period} \cdot WACC}{(1+WACC)^{depreciation\ period} - 1} = 0.0838, \quad (4)$$

With AF, the pipeline-specific expenditures (TOTEX) are calculated as

$$TOTEX = \frac{AF \cdot total\ investment + 5 \cdot total\ length}{annual\ hydrogen\ throughput}, \quad (5)$$

with TOTEX in EUR/MWh_{H2}, total investment in EUR, total length in m, and annual hydrogen throughput in MWh_{H2}/a.

2.2 Capacity Scenario and Pipeline Topologies

The capacity scenario for this study is based on an energy system design with respect to hydrogen reconversion pathways according to Welder et al. [11]. The aim of the authors' system design is to cover the positive residual load at every point in time and in every region of the German federal state of North Rhine-Westphalia (NRW) in the year 2050 by means of surplus electricity from northern Germany. The underlying residual load data from Robinius et al. [35] is used, who design a German energy system for the year 2050 with spatially resolved production and demand data to supply most of the German electricity sector with renewable energies. The major share of renewable electricity is produced from wind onshore and offshore as shown in Table 2 and is located in northern Germany, see Figure 3. Therefore, the negative residual loads are located in northern districts as well. More details about the underlying scenario like the spatially resolved installed capacities of renewable energy technologies with corresponding temporal electricity generation profiles are given in Robinius et al. [35] and Welder et al. [11].

Table 2: Renewable power scenario for Germany in 2050 according to Robinius et al. [35]

Technology	Installed capacity (GW)		Energy type	Electrical energy (TWh)
Onshore	170		Produced electricity used	381*
Offshore	59		Negative residual loads	293*
Photovoltaics	55		Remaining positive residual loads	147
Biomass	7		Total electricity demand	528
Hydropower	6			

*The potential amount of electricity produced from renewable energy is taken from the sum of the produced electricity used, the negative residual loads (surplus electricity), and power grid losses. The potential amount of electricity produced was calculated for the year 2050 using weather data from 2013.

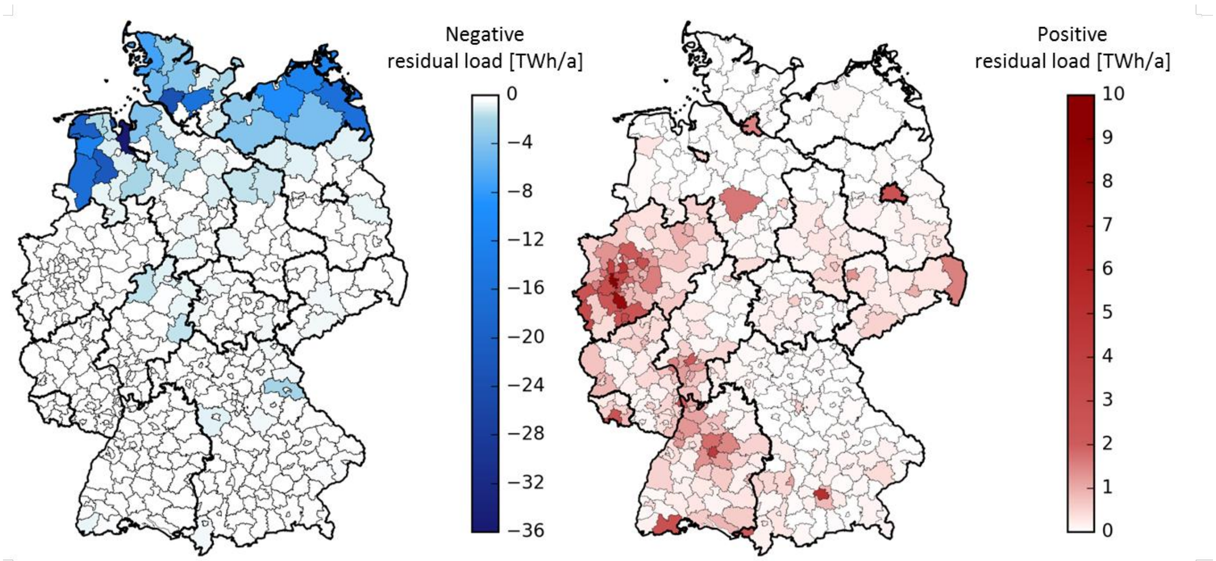

Figure 3: Negative (blue) and positive (red) residual load for Germany in 2050 based on the electricity system assumptions from Robinius et al. [35], reproduction from Emonts et al. [36], with permission from Elsevier.

Welder et al. [11] analyze hydrogen reconversion pathways for the federal state of North Rhine Westphalia with spatially- and temporally-resolved load data in which energy transfer using the necessary infrastructure (hydrogen pipelines and underground high-voltage direct-current transmission cables) is integrated in the model. The system design is shown in Figure 4.

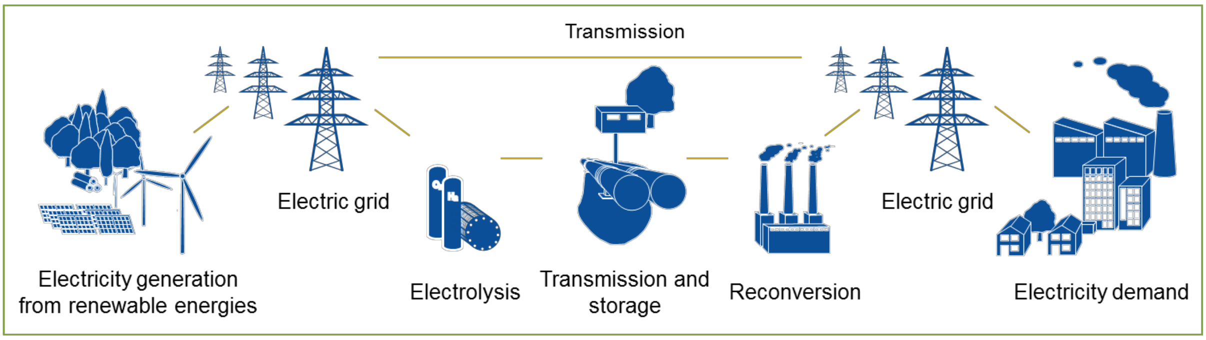

Figure 4. Schematic illustration of hydrogen reconversion pathway for supplying North Rhine Westphalia (NRW) with electricity, reproduction from Welder et al. [11], with permission from Elsevier.

As potential reconversion options, Welder et al. [11] evaluated reconversion by combined cycle gas turbines (CCGT), solid oxide fuel cells, gas motors, polymer electrolyte membrane fuel cells, and gas turbines. According to their results, electrification by means of CCGT is the most promising pathway with respect to economic boundaries. For our study, we focus on the pathway utilizing CCGT from Welder et al. [11]. In Figure 5, the resulting capacities for the CCGT pathway are visualized.

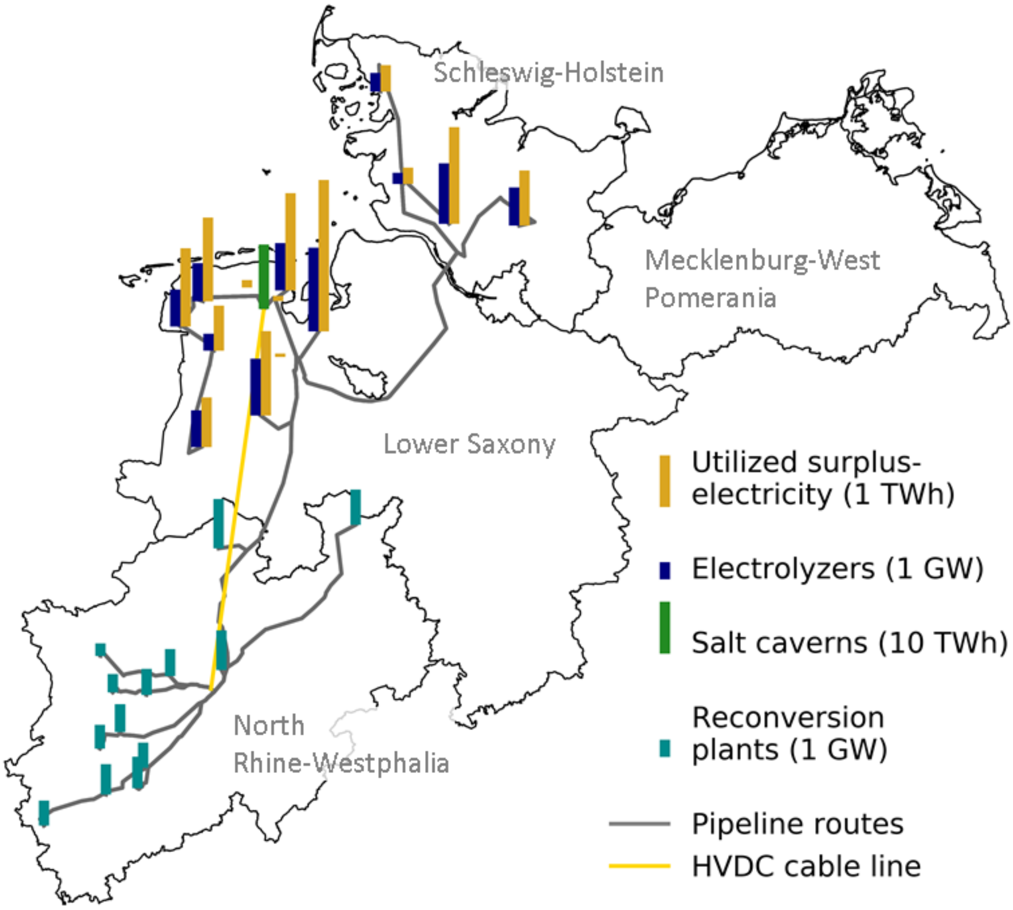

Figure 5. Installed capacities of the CCGT reconversion power plants, storage capacity of the salt caverns, surplus electricity used, and the pipeline routes, as well as HVDC routes in the cost-optimized reconversion pathway, reproduction from Welder et al. [11], with permission from Elsevier.

The pathways from Welder et al. [11] are modeled and optimized with the optimization framework FINE (Framework for Integrated Energy System Assessment) [37]. Within FINE, the hydrogen pipeline costs are integrated into the energy system optimization framework by determining the distances from all electrolysis locations to the salt cavern storage, the salt cavern storage to the centroid of NRW, and from the centroid of NRW to the CCGT locations via Dijkstra's shortest path algorithm [25]. The algorithm is utilized to route new pipelines next to existing infrastructure like the natural gas grid, motorways, and railway tracks. Based on these distances, the model is free to specify the pipeline diameters.

Even if the pipeline routes from Figure 5 look like a network merging multiple parallel pipes into single ones, the model itself does not take this into account and opts for a diameter for each connection. The shortest path distances are integrated to avoid the utilization of detour factors, but are not taking into account multiple parallel pipes. From the view of the model framework, the pipeline structure looks like that which is sketched in Figure 6, on the left side. While this star network has point-to-point connections between the key elements, the network, as shown in Figure 5, could be elaborated in much more detail by separating the pipeline routes into smaller sections and adding nodes where the pipes are forking, as is shown on the right-hand side of Figure 6, the tree network.

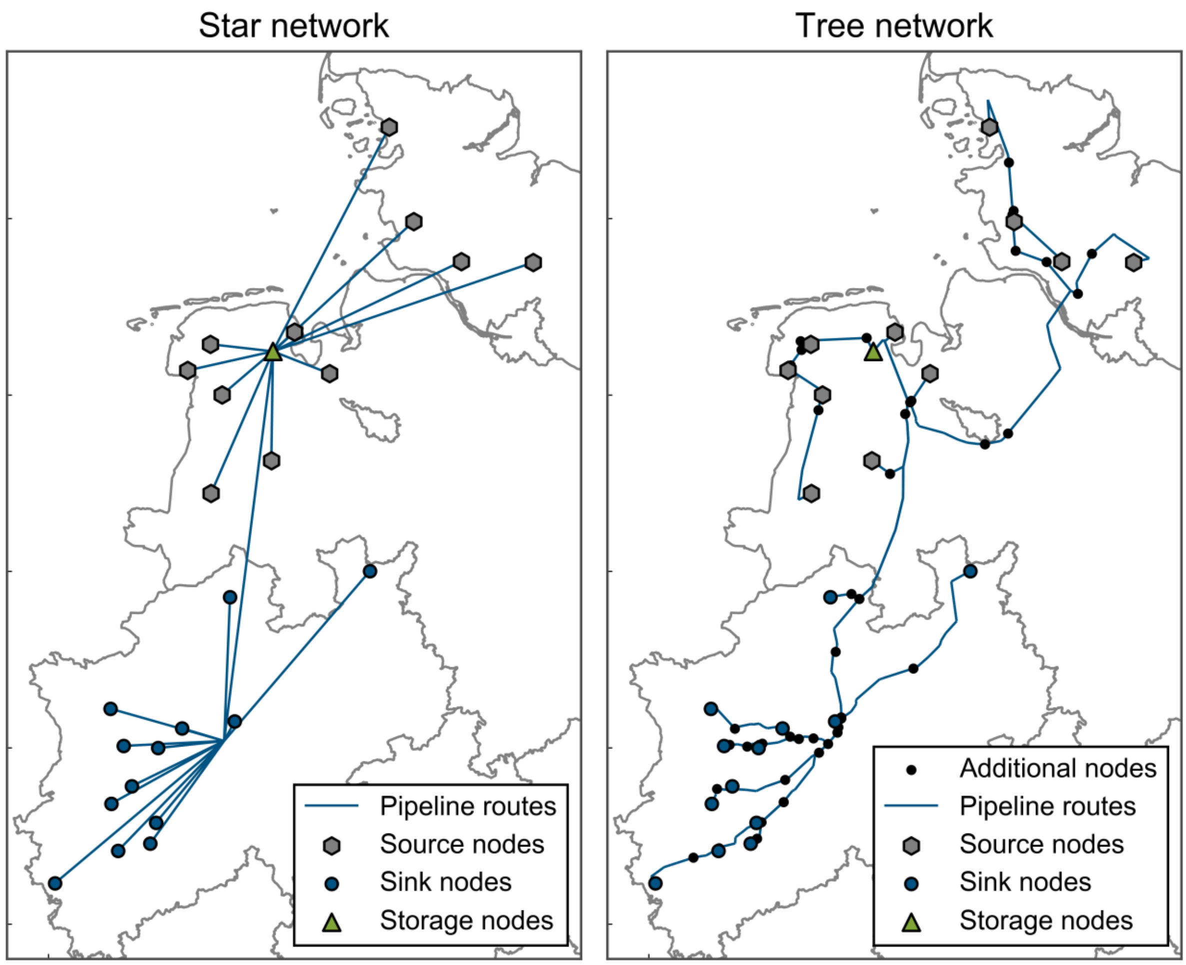

Figure 6. Model view on the pipeline network. Left: star network with connections from electrolysis to storage, from storage to the centroid of NRW, and from the centroid of NRW to power plant locations. Right: tree network with a fine pipeline grid.

2.3 Demand and Supply Scenarios

In the context of renewable energy technologies, demand and supply is affected by uncertainties such as weather conditions. Consequently, demand and supply fluctuations have to be considered. Robinius et al. [19] present an algorithm that tackles demand and supply uncertainties by constructing finitely many "robust" scenarios for a given tree-structured pipeline network. Here, "robust" means optimizing with respect to these scenarios, guaranteeing a feasible solution for all balanced demand and supply scenarios within given capacities of sources, sinks, and storage options. For the generation of these "robust" scenarios at most quadratically many (in terms of the number of nodes of the considered network), linear optimization problems must be solved, which can be done efficiently, i.e., in polynomial time. In this study, we compute the "robust" demand and supply scenarios with the help of the method presented in Robinius et al. [19] for the star network, as well as for the tree network. These scenarios form the basis of the following computational results.

3. Results and Discussion

In this section, the results for each pipeline topology as well as the linear and nonlinear fluid flow model are presented. Afterward, the results are compared and discussed.

3.1 Analysis of the Star Network

First, the spatially resolved results for the star network are shown on the left-hand side of Figure 7. These results show that for each connection, from electrolysis to the storage, as well as the connections from the centroid of NRW to the locations of the CCGT, the selected diameters remain fairly small, with DN900 being the largest. The looped connection from the storage to the centroid of NRW has by far the largest pipeline diameter, as it is the main connection between north (production) and south (demand).

Within the scenario evaluation, a scenario set of 35 different scenarios are shown to be sufficient for a robust design of the network according to Section 2.3. On the right-hand side of Figure 7, the total investment of the pipeline network separated by diameter sizes is given. For the nonlinear pressure drop approach, a total investment of 3.77 billion EUR is computed. The linear approach, according to Welder et al. [11], results in pipeline costs of 3.93 billion EUR, which represents an overestimation of roughly 3.4%. It is obvious that especially high diameters are overestimated by the linear model.

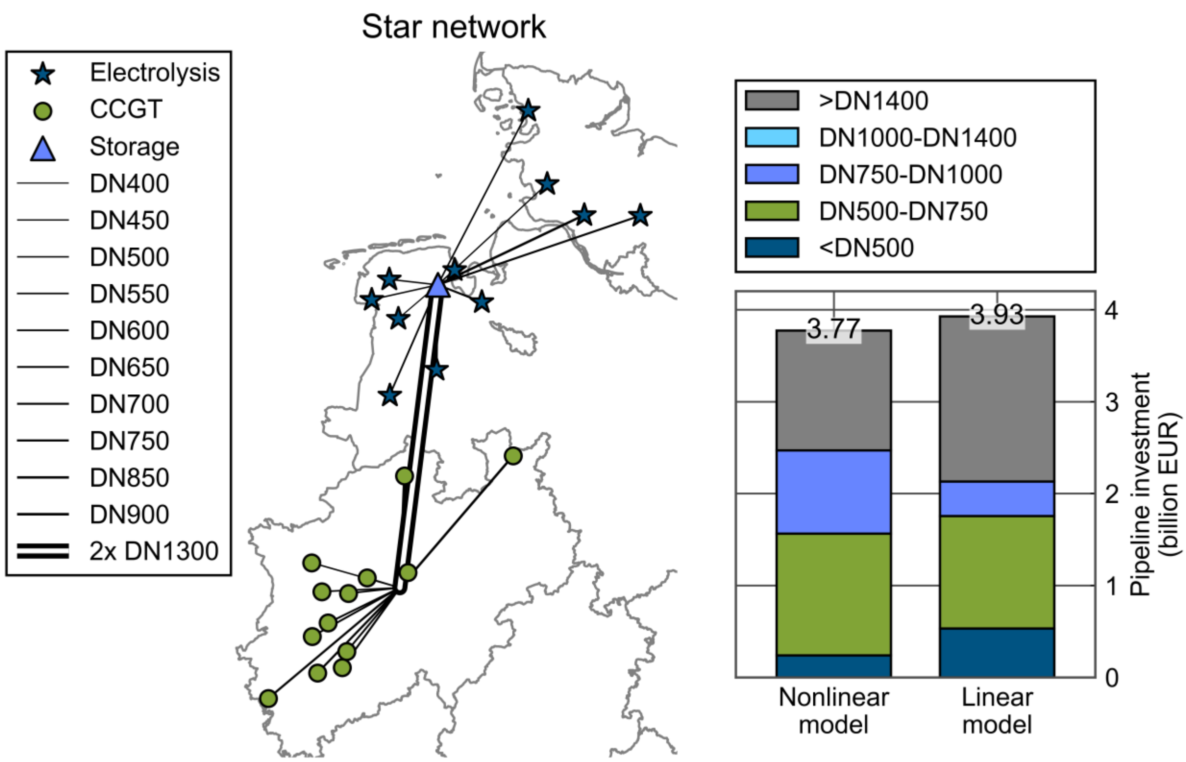

Figure 7. Spatially resolved results of the star network (left) and pipeline investment distribution separated by pipeline diameters (right).

In Figure 8, the specific pipeline investment, the maximum occurring gas velocity, and the diameters of each pipeline section are drawn depending on their maximum hydrogen flow and compared for the nonlinear and linear models. The results for low hydrogen flows are similar for the linear and nonlinear model. Only the pipe with the highest hydrogen flow, which is, according to Figure 7, the pipeline between the centroid of NRW and the storage, has a significantly lower diameter in the nonlinear model compared to the linear approach. This is justified by the pressure drop consideration that allows for higher gas velocities compared to the linear approach. The view of gas velocities exposes the reason for the cost distribution in Figure 7. Low hydrogen flow rates tend to have lower gas velocities than 10 m/s, while the velocity increases for high flow rates are up to 18 m/s.

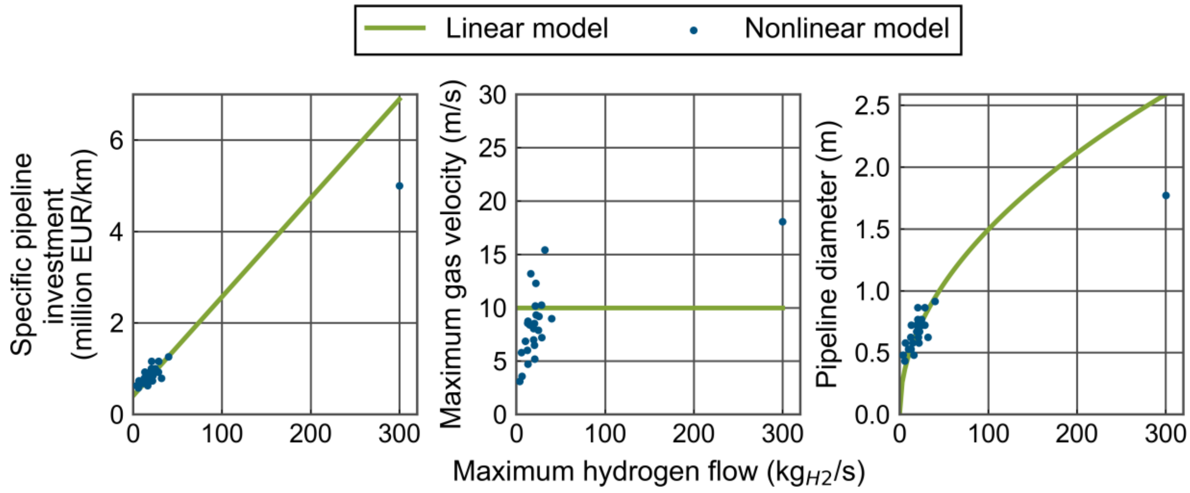

Figure 8. Specific costs, maximum gas velocities, and the diameters of each pipeline section depending on its maximum hydrogen flow in 35 scenarios for the star network results.

During the optimization, the pressure gradients for 35 scenarios are calculated to consider the pressure drop in each pipeline section. Figure 9 shows the pressure gradients of scenario 2, which has the lowest pressure difference, and scenario 21, which has the largest one. Scenario 2 only has a single connection between production and storage, which does not cause a notable hydrogen flow and therefore keeps the pressure drop low. In contrast, scenario 21 has very high demand and therefore requires a high outflow from the storage. This causes a high pressure drop on the connection from the storage to the centroid of NRW.

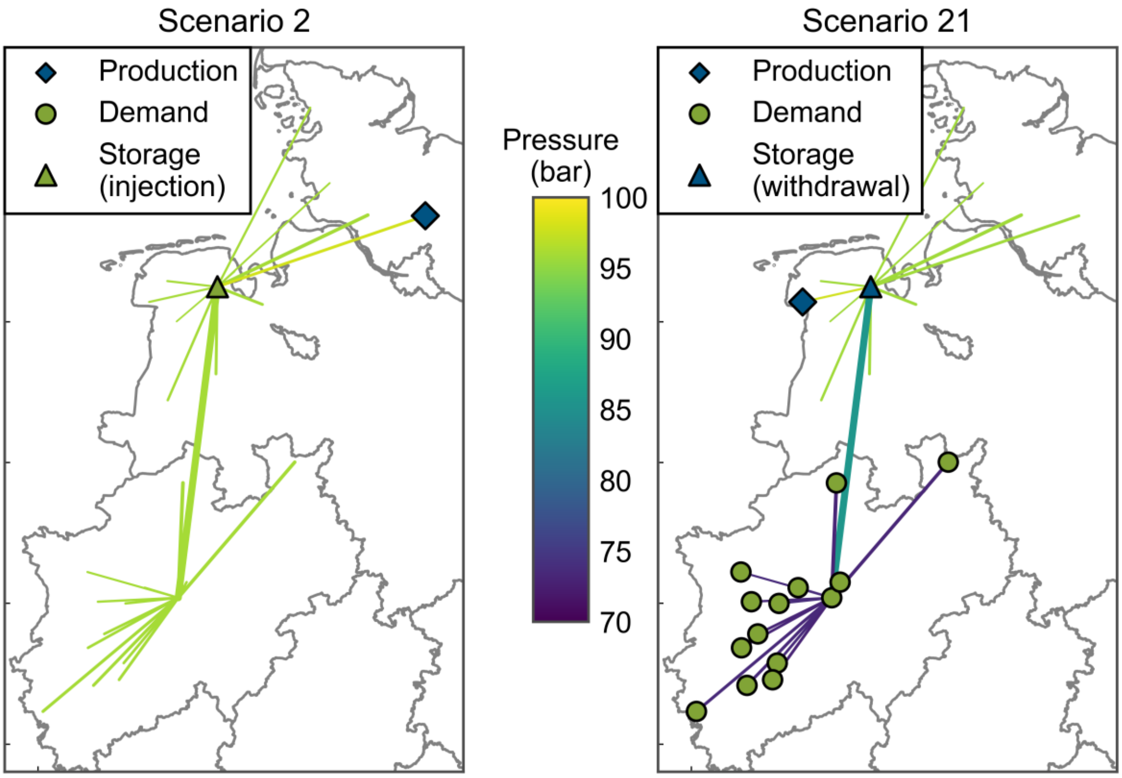

Figure 9. Exemplary pressure gradients of the star network for the low-demand scenario 2 and high-demand scenario 21.

3.2 Analysis of the Tree Network

The scenario generation resulted in 23 scenarios that are suitable for producing a robust solution for the tree network. The spatially resolved results for the tree network are shown on the left-hand side of Figure 10. The results show that there remains a main backbone pipeline, as in Figure 7, from the storage in the north to the centroid of NRW. Nevertheless, single pipes are now merged together and the cost-optimal solution shows a larger variety of selected diameters. Even pipeline diameters between DN900 and DN1400 are now selected due to the merging of specific pipes to higher diameters. Analyzing the total investment costs on the right-hand side of Figure 10, is apparent that the total costs of the pressure drop approach sums of up to 2.47 billion EUR. In contrast, the linear approach for the tree network results in 2.94 billion EUR. This represents an overestimation of costs by the linear model of 20%.

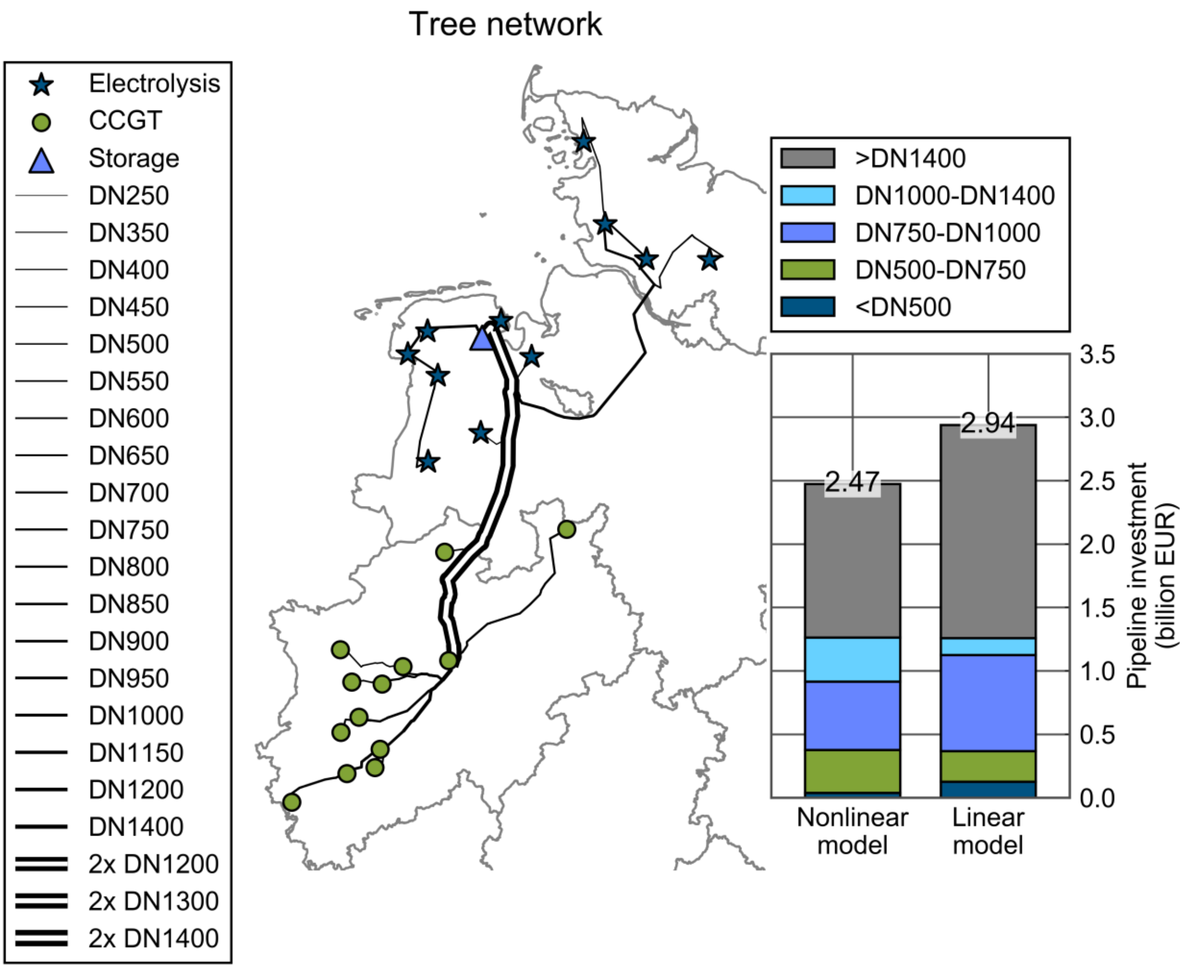

Figure 10. Spatially resolved results of the tree network (left) and pipeline investment distribution separated by the pipeline diameters (right).

Figure 11 gives insight into the reasons for the large benefit of the nonlinear pressure drop consideration. As already mentioned, there are now more pipelines with larger diameters. While the linear model selects for all pipes with the same maximum hydrogen flow the same diameter, the nonlinear model allows for different diameters. These tend to have lower specific costs compared to the linear model, as the maximum velocities are again increasing for increasing flow rates. While the maximum velocity occurring in Figure 8 is roughly 18 m/s, the maximum velocity for the tree network rises to almost 30 m/s, which is set as a limit. This is caused by having pipelines with smaller distances compared to the star network and is followed by more options for the solver to find cheaper solutions.

Figure 12 showcases the pressure gradients for the tree network of scenario 2, which has the lowest pressure difference, and scenario 3, which has the largest one. Scenario 2 has, in contrast to Figure 9, multiple locations of production that load the storage. Scenario 3 has, similarly to Figure 9, a very high demand and therefore requires a high outflow from the storage.

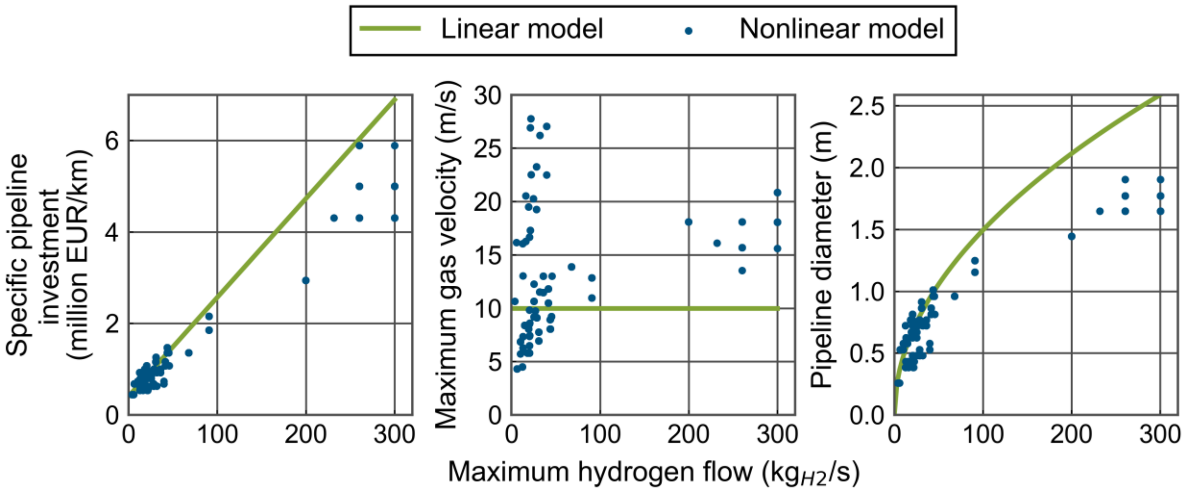

Figure 11. Specific costs, maximum gas velocities, and diameters of each pipeline section depending on its maximum hydrogen flow in 23 scenarios for the tree network results.

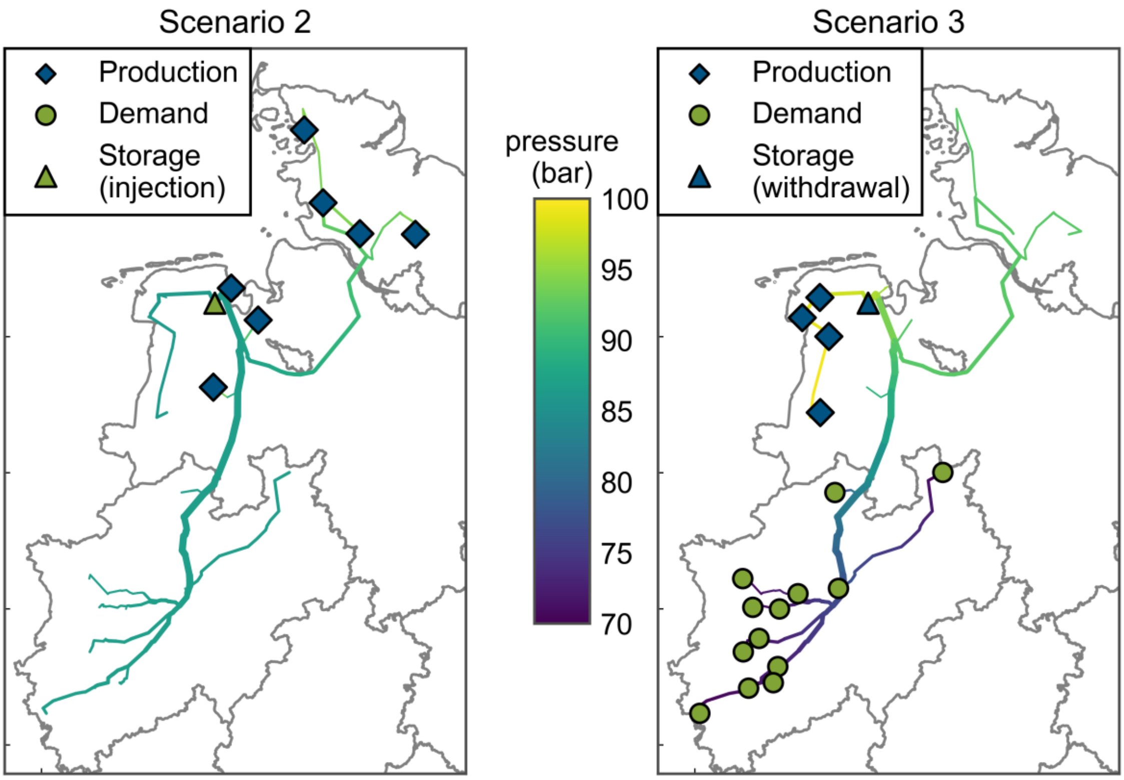

Figure 12. Exemplary pressure gradients of the tree network for scenario 2 (lowest pressure gradient) and scenario 3 (largest pressure gradient).

3.3 Comparison and Discussion

For a final comparison, Figure 13 shows the results for the total investment costs caused by both network topologies in comparison. It is obvious that the tree network assumption allows for a huge reduction in the pipeline investment requirement, even for the linear approach. This is caused by forking the network instead of using source-sink connections and is explained by Figure 2: two looped pipes of 2 GW_{H2} would account to 766 EUR/m each (1524 EUR/m in total), while a 4 GW_{H2} pipe would account for 1122 EUR/m and is, thus, 26% cheaper. The fixed cost share of 402 EUR, according to Welder et al. [11] and stated in Equation (3), especially impacts low pipeline diameters and affects every meter per pipeline built. As Figure 7 revealed, roughly 50% of the pipeline costs of the star network using the linear flow model are caused by pipelines with maximum occurring hydrogen flows below 5 GW_{H2}. In addition, bi-directional gas flows do not occur in the star network due to the topology. However, they occur within the tree network, which decreases the number of required pipes even more. These aspects lead to a large cost decrease for the linear approach from the star network to the tree network of roughly 25% of the total investment costs.

Figure 14 presents the length of the considered pipes obtained with the nonlinear model. Due to the parallel pipes consideration of the star network, the total pipeline length sums up to 3069 km, whereas 91% of this total length belongs to small diameter pipelines. The merging of these pipes in the tree network reduces the total pipeline length to 1451 km, which is only 47% of the star network's length and represents the main cost driver in Figure 13.

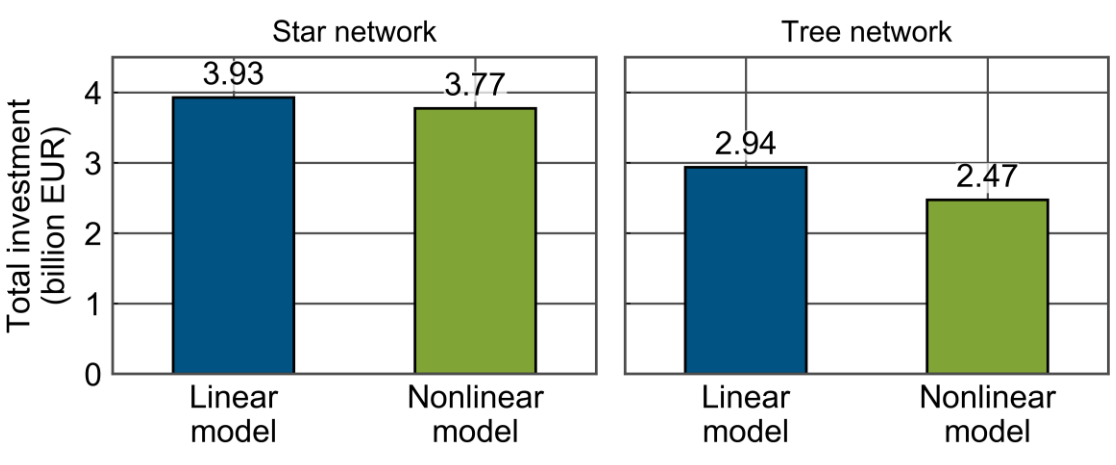

Figure 13. Comparison of pipeline investment costs for the two different networks and the two different flow modeling approaches.

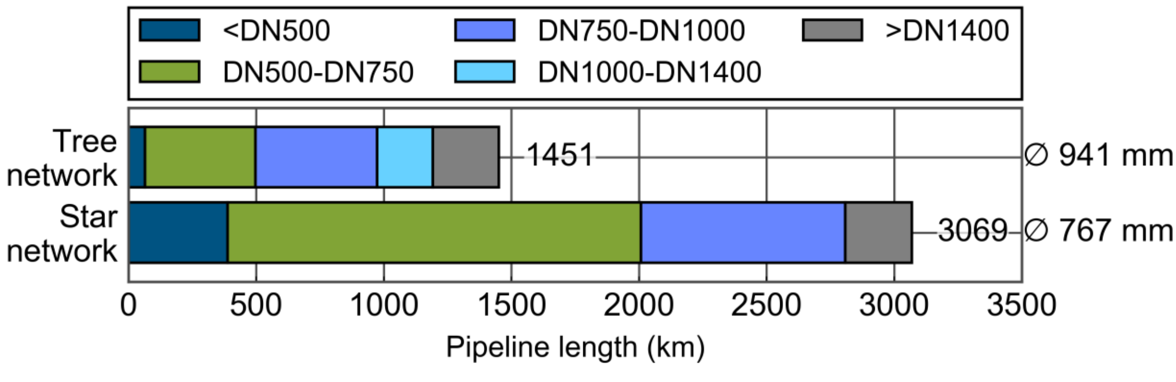

Figure 14. Comparison of the pipeline lengths of the two different networks considered.

As it is shown in Figure 8 and Figure 11, the linear approach underestimates the costs for low flow rates compared to the pressure drop approach, while larger flow rates are overestimated. With regard to the star network, the total investment is balanced out and the relative difference between the linear and nonlinear model is below 5%. In contrast, the tree network has pipelines with larger diameters instead of parallel ones. The average selected diameters of the tree network is with 941 mm higher compared to the star network with 767 mm. This overweighs the cost advantage of high diameters, as discussed in Figure 2 for the nonlinear approach and allows for a cost reduction for the tree network of an additional 16% compared to the linear model. Comparing the linear modeling applied to the star network with the nonlinear modeling in the tree network, a total cost reduction from 3.93 billion EUR to 2.47 billion EUR occurs, which amounts to 37%. This impact reveals a large reduction in the total investment requirements, keeping in mind that the distances and pipes are based on the same topology.

Furthermore, a comparison of the specific hydrogen costs caused by the pipeline is shown in Figure 15. Based on the scenario from Welder et al. [11], a total electricity demand of 51.7 TWh is produced for electrical reconversion. As the specific pipeline costs are mainly driven by the capital expenditure (CAPEX), the cost differences from the linear model on the star network compared to the nonlinear model on the tree network are roughly 37%. Comparing the specific pipeline costs with the overall electrical reconversion costs from Welder et al. [11] of 176 EUR per MWh_{el}, a fairly small impact of the pipeline costs for the entire energy system is revealed. The improvements made using the tree network, from 6.7 to 4.2 EUR/MWh, account for 1.4% of the cost reduction for the entire electrical reconversion compared to the star network.

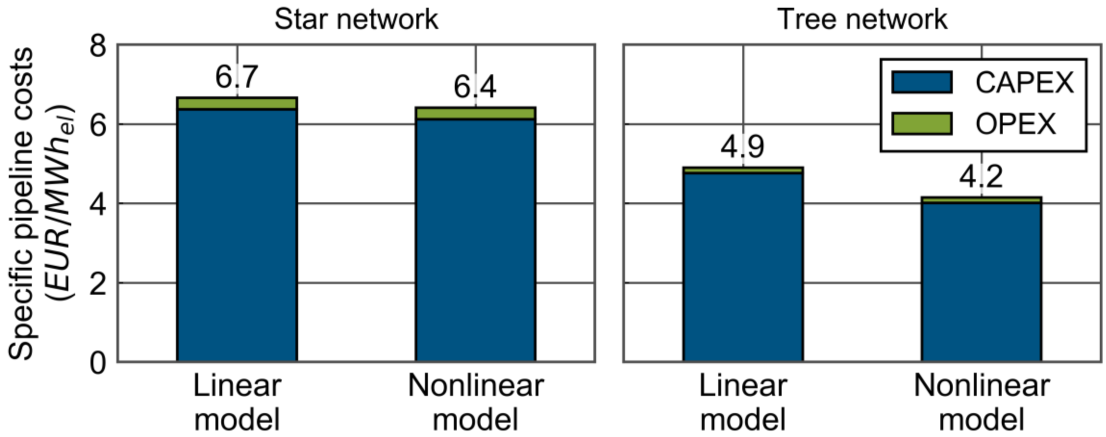

Figure 15. Comparison of specific pipeline costs for two different networks and two different flow modelling approaches. Total re-electrification costs from Welder et al. [11] for the CCGT scenario are 176 EUR/MWh_{el}.

Indeed, this result highly depends on the scenario assumptions. The overall hydrogen demand is 57 TWh of hydrogen for yearly electrical reconversion, which amounts to roughly 2.6 million tons of hydrogen per year. Reuß et al. [9] compute an overall demand of 3.03 million tons of hydrogen for supplying German passenger cars with 75% of the share of fuel cell electric vehicles. This indicates that the overall hydrogen demand in this study is high and leads to low costs. Lowering the overall demand will lead to decreased pipeline diameters and therefore higher specific costs of hydrogen [5, 9]. It should be noted though that with decreased diameters, the relative differences between the linear and nonlinear model will decline as well. To adequately analyze this issue, further considerations are necessary in future studies.

Finally, the resulting diameters obtained from the linear model are used as inputs in the nonlinear model and checked for their feasibility. To do so, the pipeline costs for the respective diameters from the linear result were set to zero. If the model opts to build a larger pipeline, the results obtained from the linear model are infeasible for the nonlinear constraints of pressure drop. In Figure 16, the results for the feasibility check of the star network and the tree network are given. In the star network, three pipes are not feasible and the pipeline diameter is increased. For the tree network, just one pipe is changed. However, none of both pipeline systems is entirely feasible. This represents an important benefit of the nonlinear model, as its results are closer to reality.

4. Conclusion

Future energy systems based on renewable energy technologies could heavily rely on hydrogen as a key element for large-scale storage, sector coupling and even electrical reconversion. Therefore, hydrogen pipelines are often used in energy system optimization models as a large-scale transport option. However, an optimized cost calculation of hydrogen flow through pipelines with respect to pressure drops is highly nonlinear and difficult to integrate into optimization models. Thus, it is often simplified in the literature. This contribution aims at evaluating the impact of this simplification on the feasibility and pipeline costs. To this end, a simplified topology from the literature is selected that is reproducible and analyzed. Based on this topology, two different network setups, namely a star network and tree network, are generated. With these two networks, two different flow modeling approaches were applied: a simplified fluid flow consideration with a fixed velocity and a cost calculation taking the pressure drop into account.

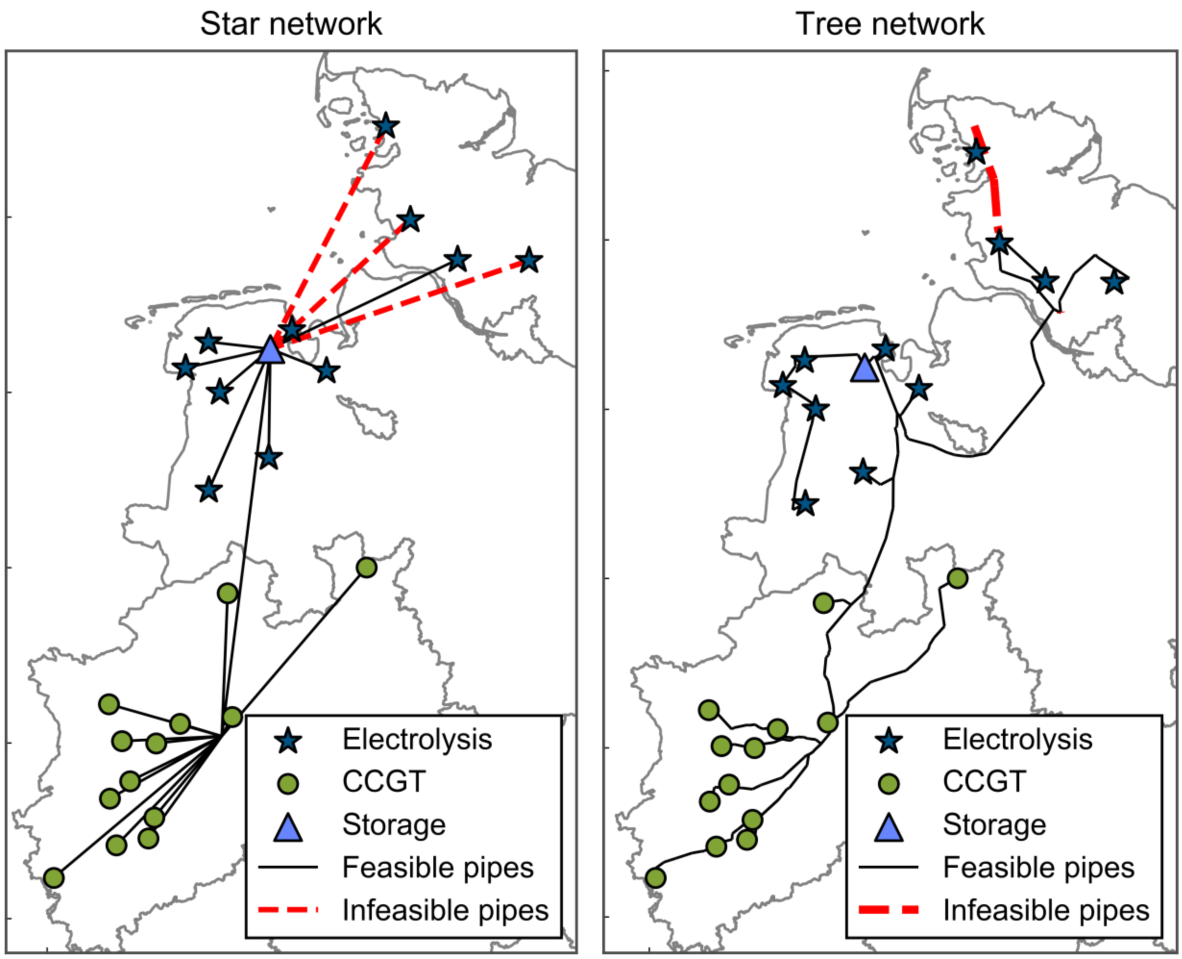

Figure 16. Feasibility check for the pipeline diameters from the linear model for the star network and the tree network with the nonlinear model.

The main result of this study is that a network with an increased number of nodes to fork pipes significantly lowers the total pipeline length, as well as the costs with the same system design approach. The consideration of a nonlinear pressure drop for the cost calculation with discrete diameters showed additional cost benefits compared to the linearized cost computation that utilizes a fixed gas velocity for the flow calculation. The differences between the assumed gas velocity and the resulting gas velocity chosen by the nonlinear model increases for larger diameters based on the obtained results. Consequently, pipelines with increasing hydrogen flows tend to be overestimated by linearizing the investment depending on the hydrogen flow. In summary, a drop of up to 37% in pipeline investment can be observed. However, the impact on the costs of electrical reconversion is almost not influenced, as the cost of renewable electricity and the respective efficiencies are significantly more expensive than the transport infrastructure. In such cases, the high computational effort for the in-depth representation of physical gas flow seems very high.

Based on these results, the utilization of nonlinear approaches for pressure drop consideration of pipeline flows, as well as increasing the number of network nodes, is relevant as it allows for the identification of the drawbacks of model simplification. However, the utilization of such approaches in energy system optimization models is always a trade-off between computational performance and the necessary degree of detail. Meanwhile, the integration of nonlinearities into energy system optimization models cannot be expected due to their high computational burden. Nevertheless, application as part of post-processing would strengthen the results and improve the credibility of future analyses. Especially for future industrial applications and the utilization of systems analysis for strategic asset planning, the credibility of overall system results will play an important role.

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Article 7

Computing technical capacities in the European entry-exit gas market is NP-hard

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ORIGINAL RESEARCH

Computing technical capacities in the European entry-exit gas market is NP-hard

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Abstract
As a result of its liberalization, the European gas market is organized as an entry-exit system in order to decouple the trading and transport of natural gas. Roughly summarized, the gas market organization consists of four subsequent stages. First, the transmission system operator (TSO) is obliged to allocate so-called maximal technical capacities for the nodes of the network. Second, the TSO and the gas traders sign mid- to long-term capacity-right contracts, where the capacity is bounded above by the allocated technical capacities. These contracts are called bookings. Third, on a day-ahead basis, gas traders can nominate the amount of gas that they inject or withdraw from the network at entry and exit nodes, where the nominated amount is bounded above by the respective booking. Fourth and finally, the TSO has to operate the network such that the nominated amounts of gas can be transported. By signing the booking contract, the TSO guarantees that all possibly resulting nominations can indeed be transported. Consequently, maximal technical capacities have to satisfy that all nominations that comply with these technical capacities can be transported through the network. This leads to a highly challenging mathematical optimization problem. We consider the specific instantiations of this problem in which we assume capacitated linear as well as potential-based flow models. In this contribution, we formally introduce the problem of Computing Technical Capacities (CTC) and prove that it is NP-complete on trees and NP-hard in general. To this end, we first reduce the Subset Sum problem to CTC for the case of capacitated linear flows in trees. Afterward, we extend this result to CTC with potential-based flows and show that this problem is also NP-complete on trees by reducing it to the case of capacitated linear flow. Since the hardness results are obtained for the easiest case, i.e., on tree-shaped networks with capacitated linear as well as potential-based flows, this implies the hardness of CTC for more general graph classes.

Keywords European entry-exit gas market · Technical capacities · Potential-based flows · Computational complexity · NP-hardness

Mathematics Subject Classification 90B10 · 90C35 · 90C60 · 90C90

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1 Introduction

The European gas market is organized as a so-called entry-exit market system, which has been the outcome of the European gas market liberalization; see Directive (1998, 2009, 2003). The main goal of the entry-exit system is to decouple the trading and transport of gas. The current market organization that should achieve this goal is mainly split into different stages in which the transmission system operator (TSO) and the gas traders interact with each other. First, the TSO is obliged to allocate so-called maximal technical capacities at all nodes of the network at which gas can be injected or withdrawn. After determining the maximal technical capacities, the TSO and the gas traders sign mid- to long-term capacity-right contracts, called bookings, in which the traders buy rights for the maximal injection or withdrawal at certain entry and exit nodes of the network. In doing so, the maximal bookable capacities are bounded from above by the maximal technical capacities. These mid- to long-term booking contracts bound the amounts of gas that traders can nominate on a day-ahead market. On this day-ahead basis, the traders nominate the amount of gas that they inject or withdraw on the next day while the nominated amount of gas is bounded above by the beforehand determined bookings. Finally, the TSO has to operate the network such that the nominated amount of gas is transported as requested. By signing the booking contract, the TSO has to guarantee the feasibility of transport for every booking-compliant nomination, i.e., every nomination below the booked capacity. Since the gas traders can sign any booking below the maximal technical capacities, the TSO has to guarantee that all technical-capacities-compliant nominations, i.e., infinitely many flow situations, can be transported through the network. Thus, computing maximal technical capacities in the European gas market leads to a challenging mathematical problem. A mathematical model of the European entry-exit gas market system that models the described market organization has been developed in Grimm et al. (2019). The model is a four-level model and it is shown that, under suitable assumptions, it can be reformulated as an equivalent bilevel model. Here, we focus on the first stage where the maximal technical capacities need to be computed. For doing so, we consider passive networks, i.e., no controllable network devices like valves or compressors exist. We further focus on stationary models of gas transport with capacitated linear flow models as well as on potential-based flows as used in, e.g., Schewe et al. (2020), Groß et al. (2019). One of the main differences between capacitated linear flows and the more accurate potential-based flow models is that, in the latter, no cyclic flows are possible. On the one hand, this provides additional structure that can be exploited for analyzing the feasibility of nominations and bookings as well as the maximization of technical capacities. However, on the other hand, the coupling between node potentials and arc flows usually is nonlinear and thus, leads to a harder class of optimization problems.

Mathematical optimization methods for gas transport networks have been studied with great interest in the last decades. For a comprehensive overview of this field see, e.g., the book (Koch et al. 2015) and the survey article (Ríos-Mercado and Borraz-Sánchez 2015) as well as the references therein. Most of the literature focuses on checking the feasibility of a single nomination as well as its transport through the network. In Bakhouya and De Wolf (2007) and De Wolf and Smeers (2000), the cost-optimal gas transport in the Belgian network before and after the European market liberalization is discussed. In these papers, the gas physics is approximated by piecewise-linear functions, leading to mixed-integer linear programs (MILPs). Alternative approaches that are also based on MILP techniques can be found in Geißler (2011), Geißler et al. (2013), Martin et al. (2006). Further, purely continuous and physically accurate nonlinear optimization models are, e.g., studied in Schmidt et al.

(2015a, b, 2016). Even more sophisticated nonlinear mixed-integer models are considered, e.g., in Geißler et al. (2015, 2018), Humpola (2017). Checking the feasibility of a nomination considering a capacitated linear flow model is in P, since the task can be modeled as a linear program. Additionally, the same holds in case of potential-based networks; see Collins et al. (1978), Maugis (1977). In case of networks with active elements, deciding the feasibility of a nomination is NP-hard for the potential-based flow model; see Szabó (2012).

In contrast to the rich literature on nominations, there is much less published research on the feasibility of bookings. Deciding the feasibility of a given booking consists of checking the feasibility of all booking-compliant nominations, i.e., of all infinitely many nominations within the given booking bounds. Thus, this problem can also be seen as a two-stage or adjustable robust optimization problem, see, e.g., Ben-Tal and El Ghaoui (2009), where the uncertainty set is given by the booking-compliant nominations. First results about the mathematical analysis of bookings are obtained in the PhD theses (Hayn 2016; Willert 2014). Moreover, the reservation-allocation problem studied in Fügenschuh et al. (2014) is also related to the feasibility of bookings. Considering the robust side, a set containment approach to decide the robust feasibility and infeasibility of bookings with an application to the Greek gas transport network is studied in Aßmann et al. (2018). In general, structural properties such as (non-)convexity and star-shapedness of the set of feasible nominations and bookings for different gas transport models are considered in Schewe et al. (2020). For networks consisting of pipes only together with potential-based flows, the feasibility of bookings can be characterized by conditions on nominations with maximal potential difference; see Labbé et al. (2020). Further, there it is shown that in case of a linear potential-based flow model, this characterization enables us to check the feasibility of a booking in polynomial time. Additionally, this is also possible in case of nonlinear potential-based flows in tree-shaped networks; see Labbé et al. (2020), Robinius et al. (2019). Using special structures of the nomination with maximal potential difference together with techniques from real algebraic geometry enables the authors of Labbé et al. (2019) to show that checking the feasibility of a booking in a single cycle network is in P. For the general case, i.e., a nonlinear potential-based flow model on arbitrary networks, the complexity of checking the feasibility of a booking is not yet decided and an open question for research. In the linear case, deciding the feasibility of a booking is shown to be in coNP in Labbé et al. (2020), Hayn (2016). For the case of a capacitated linear flow model, checking the feasibility of a booking is coNP-complete for cyclic networks, but it can be solved in polynomial time for trees; see Hayn (2016). An illustrative overview about the computational complexity of checking the feasibility of a booking is given in Section 6 of Labbé et al. (2020).

For computing maximal technical capacities as introduced in, e.g., Martin et al. (2011), there is much less in the literature compared to the results for nominations and even less compared to the feasibility of bookings. First results about technical capacities are again obtained in the PhD theses Willert (2014), Hayn (2016). Further, for the case of a capacitated linear flow model, exponential upper bounds for computing technical capacities are given in Hayn (2016).

Our contribution is the following. We prove that computing maximal technical capacities is NP-complete for capacitated linear flows as well as potential-based flow models even in tree-shaped networks. The proof is obtained by reducing the Subset Sum problem to computing maximal technical capacities for capacitated linear flows on trees. Afterward, we reduce computing maximal technical capacities with potential-based flows to the case of capacitated linear flows. Consequently, computing maximal technical capacities is significantly harder than checking the feasibility of bookings, since the latter can be done in polynomial time on trees. Note that our complexity results are obtained on trees. Thus, computing technical

Table 1 Complexity of computing technical capacities for different flow models (capacitated linear flow (lin.), linear potential-based (lin. pot.), and nonlinear potential-based (nonlin. pot.)) and different graph classes (trees vs. general graphs)

Graph	Flow model	Complexity	References Membership in NP	NP -hardness
Tree	lin.	NP-complete	Hayn (2016, Prop. 3.2.7)	Theorem 3.19
Tree	lin. pot.	NP-complete	Labbé et al. (2019, Thm. 12), Robinius et al. (2019, Thm. 4)	Theorem 4.10
Tree	nonlin. pot.	NP-complete	Labbé et al. (2019, Thm. 20), Robinius et al. (2019, Thm. 4)	Theorem 4.9
General	lin.	NP-hard		Theorem 3.19, Hayn (2016) (implicit)
General	lin. pot.	NP-complete	Labbé et al. (2019, Thm. 12)	Theorem 4.10
General	nonlin. pot.	NP-hard		Theorem 4.9

capacities remains hard on more complex graph classes like on general graphs. We summarize our contribution, together with a review of the results from the literature, in Table 1.

The remainder of this paper is structured as follows. In Sect. 2, the problem of computing maximal technical capacities is formally defined. The NP -completeness of computing maximal technical capacities for capacitated linear flow models on trees is shown in Sect. 3. Afterward, in Sect. 4 we extend this result by showing that this problem is also NP-complete for potential-based instead of capacitated linear flows. Finally, we close with a conclusion in Sect. 5.

2 Problem description

In general, our problem description follows the one in Labbé et al. (2019). We consider a directed and connected graph $G = (V, A)$ with nodes V and arcs A. The set of nodes is partitioned into the set V_+ of entry nodes, at which gas is supplied, the set V_- of exit nodes, where gas is withdrawn, and the set V_0 of the remaining inner nodes. We abbreviate the set $V_+ \cup V_-$ by V_b. The node types are also encoded in a vector $\sigma = (\sigma_u)_{u \in V}$ defined by

$$\sigma_u = \begin{cases} 1, & \text{if } u \in V_+, \\ -1, & \text{if } u \in V_-, \\ 0, & \text{if } u \in V_0. \end{cases}$$

We now introduce basic definitions that we use in the following.

Definition 2.1 A *load flow* is a vector $\ell = (\ell_u)_{u \in V} \in \mathbb{R}^V_{\geq 0}$, with $\ell_u = 0$ for all $u \in V_0$. The set of load flow vectors is denoted by L.

A load flow thus corresponds to an actual situation at a single point in time by specifying the amount of gas that is supplied (ℓ_u for $u \in V_+$) or withdrawn (ℓ_u for $u \in V_-$). Since we only consider stationary flows, we need to impose that the supplied amount of gas equals the withdrawn amount, which leads to the definition of a nomination.

Definition 2.2 A *nomination* is a balanced load flow ℓ, i.e., $\sigma^\top \ell = 0$. The set of nominations is given by $N{:=}\{\ell \in L : \sigma^\top \ell = 0\}$.

Nominations and bookings are connected as follows.

Definition 2.3 A *booking* is a vector $b = (b_u)_{u \in V} \in \mathbb{R}^V_{\geq 0}$, with $b_u = 0$ for all $u \in V_0$. A nomination ℓ is called *booking-compliant* w.r.t. the booking b if $\ell \leq b$ holds, where "$\leq$" is meant component-wise. The set of booking-compliant (or b-compliant) nominations is given by $N(b){:=}\{\ell \in N : \ell \leq b\}$.

Obviously, $N(b) \subseteq N \subseteq L$ holds for finite b.

We now define *feasible nominations* and *feasible bookings*, where "feasible" is meant w.r.t. technical, physical, and legal constraints of gas transport. To this end, let $c_{\mathcal{E}}(x; \ell) = 0$ and $c_{\mathcal{I}}(x; \ell) \geq 0$ be the possibly nonlinear, nonconvex, and nonsmooth constraints that model the full problem of gas transport.

Definition 2.4 A nomination $\ell \in N$ is *feasible* if a vector $x \in \mathbb{R}^n$ exists such that

$$c_{\mathcal{E}}(x; \ell) = 0, \quad c_{\mathcal{I}}(x; \ell) \geq 0 \tag{1}$$

holds. The set of feasible nominations is denoted by F_N.

We note that the set of feasible nominations F_N depends on the chosen model of gas transport. The only constraint that we need in all formulations is mass conservation at each node of the network, i.e.,

$$\sum_{a \in \delta^{\text{out}}(u)} q_a - \sum_{a \in \delta^{\text{in}}(u)} q_a = q_u \quad \text{for all } u \in V, \tag{2}$$

where $q_u \geq 0$ for entries, $q_u \leq 0$ for exits, and $q_u = 0$ for inner nodes.

The dependence of the feasible set defined in (1) on the nomination is given by a fixation of the entry and exit flows according to the nomination ℓ, i.e.,

$$q_u = \ell_u \quad \text{for all } u \in V_+, \quad q_u = -\ell_u \quad \text{for all } u \in V_-.$$

These constraints are part of $c_{\mathcal{E}}(x; \ell) = 0$ in (1).

For a nomination $\ell \in N$, we say that $q \in \mathbb{R}^A$ is an ℓ-flow if and only if q satisfies Condition (2). We note that to check whether a given nomination is feasible may lead to a nonlinearand nonconvex problem depending on the constraints $c_{\mathcal{E}}$ and $c_{\mathcal{I}}$. For more information on this problem, see, e.g., Koch et al. (2015), Pfetsch et al. (2015) and the references therein.

Definition 2.5 We say that a booking b is *feasible* if all booking-compliant nominations $\ell \in N(b)$ are feasible. The set of feasible bookings is denoted by F_B.

Due to the liberalization of the European gas market, trading and transport are decoupled. This is mainly ensured by the so-called technical capacities. The TSO is obliged to allocate such capacities while guaranteeing the feasibility of transport for any balanced injections at entry nodes and withdrawals at exit nodes within these capacities.

Definition 2.6 *Technical capacities* are a vector $q^{\text{C}} = (q^{\text{C}}_u)_{u \in V} \in \mathbb{R}^V_{\geq 0}$ with $q^{\text{C}}_u = 0$ for $u \in V_0$. The set of technical capacities is denoted by C.

We note that technical capacities q^{C} can also be seen as a booking.

Definition 2.7 We say that technical capacities q^{C} are *feasible* if all bookings $b \in B$ with $b \le q^{\mathrm{C}}$ are feasible. The set of feasible technical capacities is denoted by F_{C}.

From the previous definitions it follows that given technical capacities $q^{\mathrm{C}} \in C$ are feasible if and only if all nominations $\ell \in N(q^{\mathrm{C}})$ are feasible.

In the following, we analyze the complexity of computing maximal feasible technical capacities for different Constraints (1) of gas transport. To avoid unbounded technical capacities, we require that feasible technical capacities satisfy the conditions

$$\sum_{u \in V_-} q_u^{\mathrm{C}} \ge q_w^{\mathrm{C}}, \quad w \in V_+, \tag{3a}$$

$$\sum_{u \in V_+} q_u^{\mathrm{C}} \ge q_w^{\mathrm{C}}, \quad w \in V_-. \tag{3b}$$

Conditions (3a) ensure that for every entry node, a technical-capacities-compliant nomination exists such that the entry supplies its total capacity to the grid, i.e., a nomination $\ell \in N(q^{\mathrm{C}})$ with $\ell_w = q_w^{\mathrm{C}}$ exists. Consequently, the complete capacity of an entry node can be nominated in a nomination. In analogy, Conditions (3b) ensure that for every exit node a technical-capacities-compliant nomination exists such that the exit demands its total capacity. Conditions (3) ensure that we do not allocate "unusable" node capacities, i.e., capacities that are not completely used in any technical-capacities-compliant nomination. This prevents that the problem of computing technical capacities is unbounded by setting a single technical capacity to an arbitrary large value and the remaining capacities to zero. The latter technical capacities only contain the zero nomination as technical-capacities-compliant nomination which is usually feasible.

We finally describe the problem of computing (optimal) technical capacities for a fixed weight vector $d \in \mathbb{R}^V$ by

$$\max \quad d^\top q^{\mathrm{C}} \quad \text{s.t.} \quad q^{\mathrm{C}} \text{ are feasible technical capacities that satisfy (3).} \tag{4}$$

Note that feasibility of (4) implicitly contains feasibility of the actual flows of every technical-capacities-compliant nomination; see (1). Moreover, let us briefly discuss that Problem (4) is slightly more general than the problem that TSOs actually face in practice. The reason is that we consider arbitrary weight vectors $d \in \mathbb{R}^V$, whereas these may be restricted to be nonnegative in practice. The proof of our complexity result is already rather technical without this restriction. Thus, we keep the assumption $d \in \mathbb{R}^V$ throughout the paper and postpone the nonnegative case to future research.

We define two variants of CTC as the threshold problem associated with optimization problem (4). Note that the used specific constraints $c_{\mathcal{E}}^{\mathrm{lin}}(x; \ell)$ and $c_{\mathcal{I}}^{\mathrm{lin}}(x; \ell)$ as well as $c_{\mathcal{E}}^{\mathrm{pot}}(x; \ell)$ and $c_{\mathcal{I}}^{\mathrm{pot}}(x; \ell)$ will be specified in detail later.

Computing Technical Capacities (CTC) –capacitated linear flows.

Input:	Graph $G = (V, A)$ with entries V_+, exits V_-, inner nodes V_0, constraints $c_{\mathcal{E}}^{\mathrm{lin}}(x; \ell)$ and $c_{\mathcal{I}}^{\mathrm{lin}}(x; \ell)$, arc flow bounds $q_a^- \le q_a^+$, $q_a^-, q_a^+ \in \mathbb{Q}$ for all $a \in A$, a weight vector $d \in \mathbb{Q}^V$, and threshold value $T \in \mathbb{Q}_+$.
Question:	Do feasible technical capacities $q^{\mathrm{C}} \in F_{\mathrm{C}}$ with $d^\top q^{\mathrm{C}} \ge T$ exist?

Computing Technical Capacities (CTC) – potential-based flows.
Input: Graph $G = (V, A)$ with entries V_+, exits V_-, inner nodes V_0,
constraints $c_{\mathcal{E}}^{\text{pot}}(x; \ell)$ and $c_{\mathcal{I}}^{\text{pot}}(x; \ell)$,
potential bounds $p_u^- \leq p_u^+$, $p_u^-, p_u^+ \in \mathbb{Q}_+$ for all $u \in V$,
a weight vector $d \in \mathbb{Q}^V$, and threshold value $T \in \mathbb{Q}_+$.
Question: Do feasible technical capacities $q^{\mathrm{C}} \in F_{\mathrm{C}}$ with $d^\top q^{\mathrm{C}} \geq T$ exist?

3 Computing technical capacities for capacitated linear flows

As in the last section, we follow the notation introduced in Labbé et al. (2019). In the remainder of the paper, we focus on tree-shaped networks and thus assume that the graph $G = (V, A)$ is a tree.

We first introduce some notation. We choose to use directed graphs to represent gas networks. This modeling choice allows us to interpret the direction of flows. However, actual physical flow in a gas network is not influenced by the direction of the arcs. Thus, for $u, v \in V$, we introduce the so-called *flow-path* $P := P(u, v) = (V(u, v), A(u, v))$ in which $V(u, v) \subseteq V$ contains the nodes of the path from u to v in the undirected version of the graph G and $A(u, v) \subseteq A$ contains the corresponding arcs of this path. Moreover, we call $P(u, v)$ a directed flow-path from u to v if $P(u, v)$ is a directed path from u to v in G. For another pair of nodes $u', v' \in V$, we say that $P(u', v')$ is a *flow-subpath* of $P(u, v)$ if $P(u', v') \subseteq P(u, v)$, i.e., $V(u', v') \subseteq V(u, v)$ and $A(u', v') \subseteq A(u, v)$ holds, and if $P(u', v')$ is itself a flow-path. In particular, this allows us to define an order on the nodes of a flow-path. For $P = P(u, v)$ and $u', v' \in V(u, v)$, we define $u' \preceq_P v'$ if and only if a flow-subpath $P(u, u') \subseteq P(u, v')$ exists. If $u' \neq v'$ holds, we write $u' \prec_P v'$.

We note that if we reverse arcs in G, then ℓ-flows can be adapted by switching the sign for flows on each arc with different orientation. For a given ℓ-flow q, we say that node $u \in V$ *supplies* node $v \in V \setminus \{u\}$ if for each arc $a = (i, j) \in A(u, v)$, the conditions

$$i \prec_P j \implies q_a > 0, \quad j \prec_P i \implies q_a < 0$$

hold. We now introduce two sub-graphs for an arc $a = (u, v) \in A$. If we delete arc a in G, then the tree decomposes into two sub-trees. We define the sub-tree that includes node u as $G_u = (V_u^{(u,v)}, A_u^{(u,v)})$ and the other sub-tree that contains v as $G_v = (V_v^{(u,v)}, A_v^{(u,v)})$. By construction, $V_v^{(u,v)} = V \setminus V_u^{(u,v)}$ holds. Note that considering the reversed arc (v, u) does not change the sub-trees G_u and G_v.

We now present the capacitated linear flow model considered in this section. We consider lower and upper flow bounds $q_a^- \leq q_a^+$ that are given for every arc $a \in A$ and assume no other flow constraints. This means, we consider a standard capacitated linear flow model. Consequently, for a nomination $\ell \in N$, Constraints (1) are given by (2) and the flow bounds

$$q_a^- \leq q_a \leq q_a^+ \quad \text{for all } a \in A, \tag{5}$$

i.e.,

$$c_{\mathcal{I}}^{\text{lin}}(x; \ell) = (c_{\mathcal{I},a}^{\text{lin}}(q))_{a \in A}, \quad c_{\mathcal{I},a}^{\text{lin}}(q) = (q_a - q_a^-, q_a^+ - q_a)$$

and $c_{\mathcal{E}}$ stays the same as in Sect. 2, i.e.,

$$c_{\mathcal{E}}^{\text{lin}}(x; \ell) = (c_{\mathcal{E},u}^{\text{lin}}(q; \ell))_{u \in V}, \quad c_{\mathcal{E},u}^{\text{lin}}(q; \ell) = \sum_{a \in \delta^{\text{out}}(u)} q_a - \sum_{a \in \delta^{\text{in}}(u)} q_a - \sigma_u \ell_u.$$

We note that checking the feasibility of a nomination $\ell \in N$ w.r.t. Conditions (1) of this section is a standard ℓ-transshipment problem; see, e.g., Chapter 11 of the book (Schrijver 2003).

We first show that we can validate the feasibility of given technical capacities for a tree-shaped network in polynomial time. Afterward, in Sect. 3.2 we prove that CTC for capacitated linear flows is NP-hard even for trees.

3.1 Checking feasibility of technical capacities

Due to the tree structure of the graph, we know that for every nomination $\ell \in N$, there exists a unique ℓ-flow.

Lemma 3.1 (Lemma 1 in Robinius et al. (2019)) *Let $\ell \in N$ be a nomination. Then, a unique ℓ-flow exists and this flow can be computed in $O(|V|)$.*

With the next lemma, we bound the arc flow for a given ℓ-flow in dependence of the technical capacities by using the uniqueness of the flow-path between two nodes. Thus, the arc flow is bounded by the minimum of the aggregated capacities of the entries on one side of the arc and of the aggregated capacities of the exits on the other side of the arc.

Lemma 3.2 *Let $q^C \in C$ be technical capacities, $\ell \in N(q^C)$ a nomination, and q its unique ℓ-flow. Then, for every arc $a = (u, v) \in A$, the flow q_a is bounded by*

$$\begin{aligned} \xi_a^-(q^C) := -\min\left\{ \sum_{w \in V_+ \cap V_v^{(u,v)}} q_w^C, \sum_{w \in V_- \cap V_u^{(u,v)}} q_w^C \right\} &\le q_a, \\ q_a \le \min\left\{ \sum_{w \in V_+ \cap V_u^{(u,v)}} q_w^C, \sum_{w \in V_- \cap V_v^{(u,v)}} q_w^C \right\} &=: \xi_a^+(q^C). \end{aligned} \tag{6}$$

Proof The claim follows from the tree structure of G, Lemma 3.1, and the flow conservation constraints (2) that are satisfied by q. □

With an adaption of the approach developed in Robinius et al. (2019), we can show that the lower and upper arc flow bounds (6) are tight w.r.t. $N(q^C)$. This means that for every arc at least one nomination exists such that the corresponding flow is at the bound. To this end, we state the auxiliary lemma that directly follows from the tree structure of G.

Lemma 3.3 *Let $u \neq w \in V$. Further, let $V_u^{(u,i)} \cap V_+ \neq \emptyset$ hold for the first arc (u, i) of the unique flow-path $P(u, w)$. Then, an entry $\tilde{u} \in V_u^{(u,i)} \cap V_+$ exists such that $P(u, w) \subseteq P(\tilde{u}, w)$ holds and additionally, no entry $\bar{u} \neq \tilde{u} \in V_u^{(u,i)}$ with $P(\tilde{u}, w) \subset P(\bar{u}, w)$ exists.*

In particular, this implies $V_{\tilde{u}}^{(\tilde{u},k)} \cap V_+ = \{\tilde{u}\}$ for the first arc $(\tilde{u}, k)$ of the unique flow-path $P(\tilde{u}, w)$.

We now show that the upper arc flow bound in (6) is tight w.r.t. $N(q^C)$. We even show a stronger result: For any node pair, a nomination with unique flows exists so that for every arc of the unique flow-path between these two nodes the arc flow is at its upper bound.

Lemma 3.4 *Let $q^C \in C$ be technical capacities and $u \neq w \in V$. Furthermore, let $P(u, w)$ be a directed flow-path from u to w. Then, a nomination $\ell \in N(q^C)$ with unique flows q*

exists such that for every arc $a = (k, l) \in A(u, w)$ *the corresponding arc flow is at its upper bound in* (6)*, i.e.,*

$$q_a = \xi_a^+(q^C) \tag{7}$$

holds for every $a \in A(u, w)$*. Additionally, we can compute this nomination* ℓ *in polynomial time.*

Proof For directly applying the results of Theorem 4 in Robinius et al. (2019) and its proof, we make the following additional assumption. If u is no entry, then we interpret u as an entry with technical capacity of zero. In analogy, if w is no exit, then we interpret w as an exit with technical capacity of zero. These assumptions do not affect the upper bound in (6). Further, let arc $(u, i) \in A(u, w)$ be the first arc of the flow-path $P(u, w)$. We distinguish between two cases.

(i) Let $V_u^{(u,i)} \cap V_+ = \{u\}$. This means that no flow can be supplied to u without using arcs of flow-path $P(u, w)$. Thus, the claim directly follows from Theorem 4 in Robinius et al. (2019) and its proof.
(ii) Let $V_u^{(u,i)} \cap V_+ \neq \{u\}$ holds. We apply Lemma 3.3 and Case 1 for $\tilde{u}$ and w. In doing so, we can w.l.o.g. assume that $P(\tilde{u}, w)$ is a directed flow-path from $\tilde{u}$ to w. Consequently, (7) is satisfied for $a \in P(\tilde{u}, w)$. Due to this and $P(u, w) \subset P(\tilde{u}, w)$, the claim follows.

We can compute the corresponding nominations of Case 1 and 2 in polynomial time due to Lemma 11 in Robinius et al. (2019). □

Using Lemma 3.4, we now prove that also the lower arc flow bound of (6) is tight.

Lemma 3.5 *Let* $q^C \in C$ *be technical capacities and* $u \neq w \in V$*. Furthermore, let* $P(u, w)$ *be a directed flow-path from* u *to* w*. Then, a nomination* $\ell \in N(q^C)$ *with unique flows* q *exists such that for every arc* $a = (k, l) \in A(u, w)$ *the corresponding arc flow is at the lower bound in* (6)*, i.e.,*

$$q_a = \xi_a^-(q^C) \tag{8}$$

holds for every $a \in A(u, w)$*. Additionally, we can compute this nomination* ℓ *in polynomial time.*

Proof We consider the graph $\tilde{G} = (V, \tilde{A})$, which is a copy of $G = (V, A)$ except that arcs of $P(u, w)$ are reversed so that $P(u, w)$ is a directed flow-path from w to u. We now apply Lemma 3.4 for w and u in $\tilde{G}$. Consequently, a nomination $\ell \in N(q^{\mathrm{C}})$ with unique ℓ-flow $\tilde{q}$ in $\tilde{G}$ exist such that for $(l, k) \in A(u, w)$, it holds

$$\tilde{q}_{(l,k)} = \xi_a^+(q^{\mathrm{C}}) = \min\left\{ \sum_{v \in V_+ \cap V_l^{(l,k)}} q_v^{\mathrm{C}}, \sum_{v \in V_- \cap V_k^{(l,k)}} q_v^{\mathrm{C}} \right\}.$$

Let q be the unique flows in G corresponding to nomination ℓ. Due to the different orientation of arc $a = (k, l)$ of $P(u, w)$ in G and $\tilde{G}$ and the tree structure of G,

$$q_{(k,l)} = -\tilde{q}_{(l,k)} = -\min\left\{\sum_{v\in V_+\cap V_l^{(l,k)}} q_v^{\mathrm{C}}, \sum_{v\in V_-\cap V_k^{(l,k)}} q_v^{\mathrm{C}}\right\}$$

$$= -\min\left\{\sum_{v\in V_+\cap V_l^{(k,l)}} q_v^{\mathrm{C}}, \sum_{v\in V_-\cap V_k^{(k,l)}} q_v^{\mathrm{C}}\right\} = \xi_a^-(q^{\mathrm{C}})$$

holds. This shows the claim. □

Using the previous two lemmas, we can efficiently check the feasibility of technical capacities.

Lemma 3.6 *Let $q^C \in C$ be technical capacities. Then, q^C are feasible technical capacities if and only if for every arc $a = (u, v) \in A$, the conditions*

$$q_a^- \leq \xi_a^-(q^C) \leq 0 \leq \xi_a^+(q^C) \leq q_a^+, \tag{9}$$

are satisfied.

Proof Let q^{C} be feasible technical capacities and $a \in A = (k, l)$ an arbitrary arc. Applying Lemmas 3.4 and 3.5 for $u = k$ and $w = l$ as well as using the feasibility of every nomination in $N(q^{\mathrm{C}})$ implies Conditions (9).

Let Condition (9) be valid. Then, q^{C} are feasible technical capacities due to Lemma 3.2. □

We finally prove that checking the feasibility of given technical capacities can be done in polynomial time.

Theorem 3.7 *Let q^C be technical capacities in a tree. Then, it can be decided in polynomial time if q^C is feasible and if it satisfies Conditions (3). In particular, this implies that CTC with capacitated linear flows on trees is in NP .*

Proof For given technical capacities, we can check Conditions (3), and for every arc, the Condition (9), in polynomial time. □

We note that the result of the previous theorem is also shown in a different way by Theorem 3.2.3 and Proposition 3.2.7 in Hayn (2016). We have proven the same result differently here because we need the special structure considered in Lemmas 3.4 and 3.5 for the potential-based case, which is not considered in Hayn (2016).

3.2 Hardness

We prove that CTC for the case of capacitated linear flows is NP-complete on trees. In the remainder of this section, we require that feasible technical capacities satisfy Definition 2.6 and Conditions (3), i.e., feasible technical capacities are always feasible for Problem (4).

In what follows, we reduce the Subset Sum problem to CTC. To this end, we consider the following variant of the Subset Sum problem.

Subset Sum (SSP).
Input: $M \in \mathbb{N}$, $Z_1, \ldots, Z_n \in \mathbb{N}$ with $Z_i \leq M$ for $i \in \{1, \ldots, n\}$, $n \geq 2$, $\sum_{i=1}^{n} Z_i \geq M$.
Question: Does $I \subseteq \{1, \ldots, n\}$ with $\sum_{i \in I} Z_i = M$ exist?

This definition of the SSP slightly deviates from the original definition in Garey and Johnson (1990). The requirements $n \geq 2$, $\sum_{i=1}^{n} Z_i \geq M$, and $Z_i \leq M$ for $i \in \{1, \ldots, n\}$ can be checked in polynomial time and, thus, the considered SSP variant is still NP-hard .

The proof is structured as follows. We first construct a CTC instance on a tree based on a given SSP instance. We then prove sufficient conditions for feasibility of a solution and show a lower bound of the objective; see Lemma 3.8. This can be used to prove that the optimal value of the CTC instance exceeds a specific threshold value if the corresponding SSP instance is feasible; see Lemma 3.9. The bulk of the proof characterizes optimal solutions of the specific CTC instance; see Lemmas 3.10–3.15. We finally use these properties to prove that if the SSP is infeasible, optimal technical capacities in the specific CTC instance do not exceed the threshold value.

For an arbitrary SSP instance, we construct an instance of (4) using capacitated linear flows as follows. The graph $G(\mathsf{SSP})$ is given by

$$V = \{o, s, t\} \cup \{h_i, v_i : i \in \{1, \ldots, n\}\},$$
$$A = \{(o, s), (t, s)\} \cup \{(o, h_i), (h_i, v_i) : i \in \{1, \ldots, n\}\}.$$

We specify entries V_+, exits V_-, and inner nodes V_0 by

$$V_+ = \{t\} \cup \{h_i : i \in \{1, \ldots, n\}\}, \quad V_- = \{s\} \cup \{v_i : i \in \{1, \ldots, n\}\}, \quad V_0 = \{o\}.$$

In the following, we use the abbreviation $\delta = (n+1)^{-1}$. We now define the lower and upper arc flow bounds q_a^-, q_a^+ for $a \in A$ in $G(\mathsf{SSP})$ as follows

$$\begin{aligned} q_{(o,s)}^- &= -\delta \leq M = q_{(o,s)}^+, \quad q_{(t,s)}^- = 0 \leq \delta = q_{(t,s)}^+, \\ q_{(o,h_i)}^- &= -Z_i \leq M + \delta - Z_i = q_{(o,h_i)}^+, \\ q_{(h_i,v_i)}^- &= 0 \leq M + \delta = q_{(h_i,v_i)}^+. \end{aligned} \tag{10}$$

These arc flow bounds satisfy $q_a^- \leq 0 \leq q_a^+$ for $a \in A$ due to $Z_i \leq M$ for $i \in \{1, \ldots, n\}$. A graphical representation of $G(\mathsf{SSP})$ is given in Fig. 1.

We denote nonnegative technical capacities by q^{C}. We note that the capacity of inner nodes is set to zero and, thus, we neglect these nodes w.r.t. technical capacities. We determine the nonzero coefficients of the weight vector d as follows:

$$d_s = (n+1)((n+1)M + 1), \quad d_t = n^2 + n d_s + 1,$$
$$d_{h_i} = -1, \quad d_{v_i} = 1, \quad i \in \{1, \ldots, n\}.$$

We note that $G(\mathsf{SSP})$ is a tree and $q^{\mathrm{C}} = 0$ are feasible technical capacities for $G(\mathsf{SSP})$ because of $q_a^- \leq 0 \leq q_a^+$ for all $a \in A$. Further, we note that for a given instance of SSP, we can build $G(\mathsf{SSP})$ in polynomial time and its coding length is polynomially bounded above by the coding length of the given SSP instance.

Due to the tree structure of $G(\mathsf{SSP})$, we can check the feasibility of technical capacities in $G(\mathsf{SSP})$ in polynomial time; see Theorem 3.7. Lemma 3.6 implies that for checking the feasibility of technical capacities in $G(\mathsf{SSP})$ we have to verify the conditions

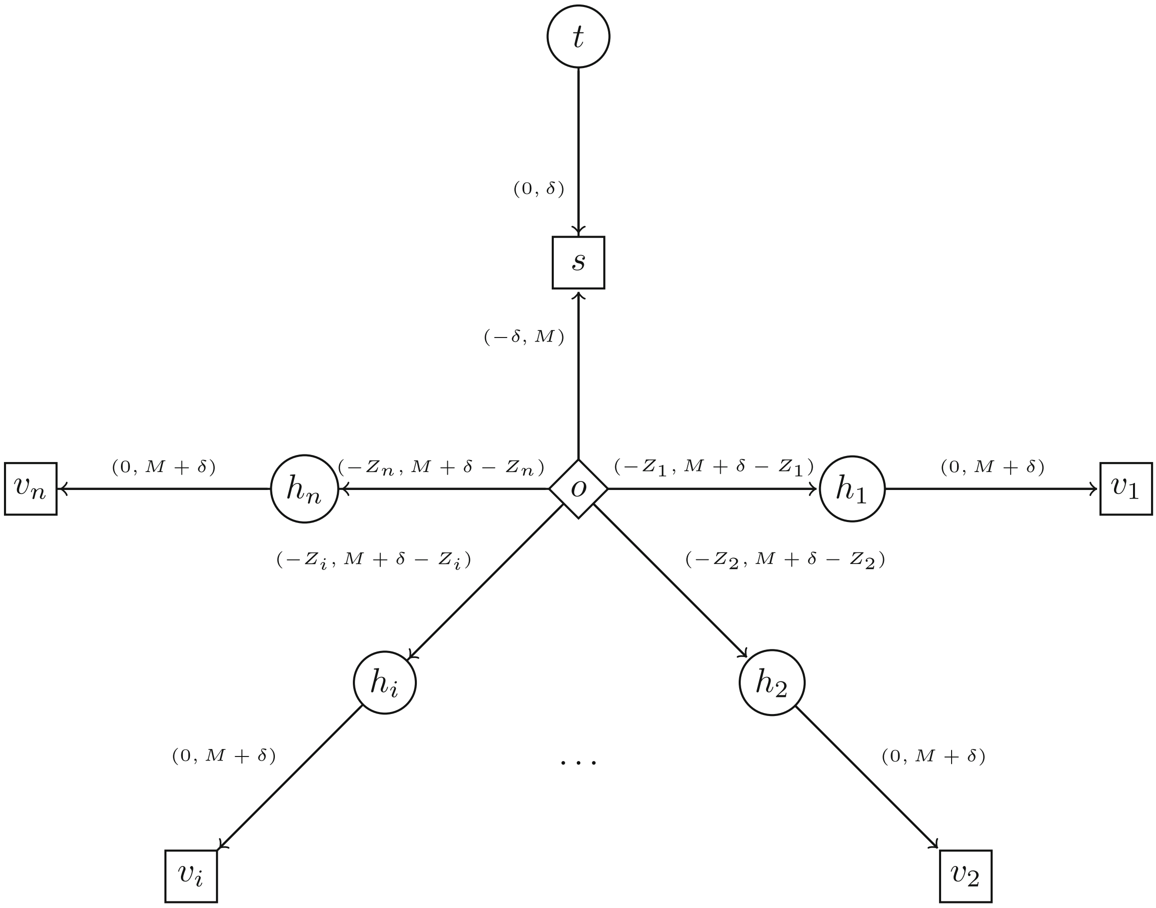

Fig. 1 The graph $G(\mathsf{SSP})$. Entry nodes are indicated by circles, exits by boxes, and inner nodes by diamonds

$$q^-_{(o,h_i)} = -Z_i \leq -\min\left\{q^{\mathrm{C}}_{h_i}, \sum_{u\in V_-\setminus\{v_i\}} q^{\mathrm{C}}_u\right\} \leq 0, \tag{11a}$$

$$0 \leq \min\left\{\sum_{u\in V_+\setminus\{h_i\}} q^{\mathrm{C}}_u,\ q^{\mathrm{C}}_{v_i}\right\} \leq q^+_{(o,h_i)} = M + \delta - Z_i, \tag{11b}$$

$$q^-_{(o,s)} = -\delta \leq -\min\left\{q^{\mathrm{C}}_t, \sum_{u\in V_-\setminus\{s\}} q^{\mathrm{C}}_u\right\} \leq 0, \tag{11c}$$

$$0 \leq \min\left\{\sum_{u\in V_+\setminus\{t\}} q^{\mathrm{C}}_u,\ q^{\mathrm{C}}_s\right\} \leq q^+_{(o,s)} = M, \tag{11d}$$

$$q^-_{(t,s)} = 0, \quad 0 \leq \min\left\{q^{\mathrm{C}}_t, \sum_{u\in V_-} q^{\mathrm{C}}_u\right\} \leq q^+_{(t,s)} = \delta, \tag{11e}$$

$$q^-_{(h_i,v_i)} = 0, \quad 0 \leq \min\left\{\sum_{u\in V_+} q^{\mathrm{C}}_u, q^{\mathrm{C}}_{v_i}\right\} \leq q^+_{(h_i,v_i)} = M + \delta \tag{11f}$$

for $i \in \{1, \ldots, n\}$.

The instance $G(\mathsf{SSP})$ is constructed in such a way that the threshold of the objective value for deciding the feasibility of SSP is given by

$$T := \sum_{i=1}^{n} (M + \delta - Z_i) + (M + \delta) d_s + d_t \delta.$$

We next prove sufficient conditions for the feasibility of technical capacities in $G(\mathsf{SSP})$.

Lemma 3.8 *Let $\tilde{q}^C \in C$ be technical capacities in $G(\mathsf{SSP})$ that satisfy the conditions*

$$\tilde{q}_t^C = \delta, \quad \tilde{q}_s^C = M + \delta, \quad \sum_{i=1}^{n} \tilde{q}_{h_i}^C = M, \quad \tilde{q}_{h_i}^C \leq Z_i, \quad i \in \{1, \dots, n\},$$

and

$$\tilde{q}_{v_i}^C = \begin{cases} M + \delta, & \text{if } \tilde{q}_{h_i}^C = Z_i, \\ M + \delta - Z_i, & \text{if } \tilde{q}_{h_i}^C < Z_i, \end{cases}$$

for $i \in \{1, \dots, n\}$. Then, $\tilde{q}^C$ are feasible technical capacities in $G(\mathsf{SSP})$ and $d^\top \tilde{q}^C \geq T - M$ holds. Furthermore, such a $\tilde{q}^C$ always exists.

Proof To construct such a $\tilde{q}^C$, one can use any fractional solution of the SSP. It is easy to verify that the capacities $\tilde{q}^C$ satisfy Conditions (3). For checking the feasibility of $\tilde{q}^C$, it is left to verify Conditions (11). Due to the construction of $\tilde{q}^C$, the Conditions (11a) and (11c)–(11f) are satisfied. For Condition (11b), we now distinguish for $i \in \{1, \dots, n\}$ two cases depending on $\tilde{q}_{h_i}^C$.

First, let $\tilde{q}_{h_i}^C = Z_i$. Consequently,

$$0 \leq \min \left\{ \sum_{u \in V_+ \setminus \{h_i\}} \tilde{q}_u^C, \ \tilde{q}_{v_i}^C \right\} = \sum_{u \in V_+ \setminus \{h_i\}} \tilde{q}_u^C = M + \delta - Z_i = q_{(o,h_i)}^+,$$

which implies Condition (11b). Second, let $\tilde{q}_{h_i}^C < Z_i$. Consequently,

$$0 \leq \min \left\{ \sum_{u \in V_+ \setminus \{h_i\}} \tilde{q}_u^C, \ \tilde{q}_{v_i}^C \right\} = \tilde{q}_{v_i}^C = M + \delta - Z_i = q_{(o,h_i)}^+,$$

which implies Condition (11b). Thus, the feasibility of $\tilde{q}^C$ follows from Lemma 3.6 and the objective value of $\tilde{q}^C$ satisfies

$$\begin{aligned} d^\top \tilde{q}^C &= -M + (M + \delta) d_s + d_t \delta + \sum_{i=1}^{n} d_{v_i} \tilde{q}_{v_i}^C \\ &\geq \sum_{i=1}^{n} (M + \delta - Z_i) - M + (M + \delta) d_s + d_t \delta = T - M. \end{aligned}$$ □

We can directly use the previous lemma to show that if the given SSP instance is feasible, then optimal technical capacities in $G(\mathsf{SSP})$ exceed the threshold value T.

Lemma 3.9 *Let the given SSP be feasible, i.e., there exists $I \subseteq \{1, \dots, n\}$ with $\sum_{i \in I} Z_i = M$. Further, let $q^C \in C$ be optimal technical capacities in $G(\mathsf{SSP})$. Then, $d^\top q^C \geq T$ holds.*

Proof Let I be a feasible solution of SSP, then we construct the following technical capacities:

$$\begin{aligned}
&\bar{q}^{\mathrm{C}}_t = \delta, && \bar{q}^{\mathrm{C}}_s = M + \delta, && \\
&\bar{q}^{\mathrm{C}}_{h_i} = Z_i, && \bar{q}^{\mathrm{C}}_{v_i} = M + \delta, && i \in I, \\
&\bar{q}^{\mathrm{C}}_{h_i} = 0, && \bar{q}^{\mathrm{C}}_{v_i} = M + \delta - Z_i, && i \in \{1, \ldots, n\} \setminus I.
\end{aligned}$$

The technical capacities $\bar{q}^{\mathrm{C}}$ are feasible because they satisfy the conditions of Lemma 3.8. Let $i \in \{1, \ldots, n\}$. We now compute the objective value of the ith branch of $G(\mathrm{SSP})$, i.e.,

$$d_{h_i} \bar{q}^{\mathrm{C}}_{h_i} + d_{v_i} \bar{q}^{\mathrm{C}}_{v_i} = -\bar{q}^{\mathrm{C}}_{h_i} + \bar{q}^{\mathrm{C}}_{v_i}. \tag{12}$$

If $i \in I$ holds, then from the construction of $\bar{q}^{\mathrm{C}}$ the ith branch (12) evaluates to

$$-\bar{q}^{\mathrm{C}}_{h_i} + \bar{q}^{\mathrm{C}}_{v_i} = -Z_i + M + \delta,$$

which also holds for $i \notin I$. Thus, the objective value of $\bar{q}^{\mathrm{C}}$ is given by

$$d^\top \bar{q}^{\mathrm{C}} = \sum_{i=1}^{n} (M + \delta - Z_i) + d_s(M + \delta) + d_t \delta = T.$$

Consequently, the claim follows because $\bar{q}^{\mathrm{C}}$ are feasible technical capacities. □

In what follows, we characterize optimal solutions; see Lemmas 3.10–3.15. Using the obtained properties we prove that if SSP is infeasible, the threshold T value is not exceeded by optimal technical capacities in $G(\mathrm{SSP})$.

We first bound the technical capacity of certain nodes.

Lemma 3.10 *Let $q^C \in C$ be optimal technical capacities in $G(SSP)$. Then,*

$$q^C_t \le \delta, \quad q^C_s \le M + \delta, \quad q^C_{v_i} \le M + \delta, \quad i \in \{1, \ldots, n\}.$$

Proof The claim follows from the explicit structure of tree $G(\mathrm{SSP})$, Conditions (3), the arc flow bounds (10), and Lemmas 3.4 and 3.5. □

Additionally, we prove that the technical capacity of entry h_i is bounded above by Z_i in an optimal solution.

Lemma 3.11 *Let $q^C \in C$ be optimal technical capacities in $G(SSP)$. Then, $q^{\mathrm{C}}_{h_i} \le Z_i$ holds for all $i \in \{1, \ldots, n\}$.*

Proof We prove the claim by contraposition, i.e., we now assume that $i \in \{1, \ldots, n\}$ with $q^{\mathrm{C}}_{h_i} > Z_i$ exists and then prove that q^{C} are not optimal technical capacities. From Condition (11a) it follows $\sum_{u \in V_- \setminus \{v_i\}} q^{\mathrm{C}}_u \le Z_i$. Thus, we obtain the bounds $q^{\mathrm{C}}_s \le Z_i$ and $q^{\mathrm{C}}_{v_j} \le Z_i$ for $j \in \{1, \ldots, n\} \setminus \{i\}$.

Using Lemma 3.10, we can bound the objective value corresponding to q^{C} from above as follows:

$$d^\top q^{\mathrm{C}} \le \delta d_t + Z_i d_s + \sum_{j=1, j \ne i}^{n} Z_i + M + \delta \le \delta d_t + Z_i d_s + nM + \delta. \tag{13}$$

For the latter inequality, we also used that $Z_i \le M$ holds. The upper bound (13) of the objective value for q^{C} and the objective value of the feasible point in Lemma 3.8 show that q^{C} is not optimal. □

We next prove that the optimal technical capacity of entry t is at its upper bound δ.

Lemma 3.12 *Let $q^{\mathrm{C}} \in C$ be optimal technical capacities in $G(SSP)$. Then, $q_t^{\mathrm{C}} = \delta$ holds.*

Proof Let q^{C} be feasible technical capacities. Due to Lemma 3.10, $q_t^{\mathrm{C}} \leq \delta$ holds. We now prove the claim by contraposition, i.e., we show that if $q_t^{\mathrm{C}} < \delta$ holds, then we can construct a better solution $\bar{q}^{\mathrm{C}}$. We set $\varepsilon \geq 0$ such that $q_t^{\mathrm{C}} + \varepsilon = \delta$ holds and construct a new solution $\bar{q}^{\mathrm{C}}$ by

$$\bar{q}_t^{\mathrm{C}} = q_t^{\mathrm{C}} + \varepsilon, \quad \bar{q}_s^{\mathrm{C}} = \max\left\{q_s^{\mathrm{C}} - n\varepsilon, \max_{u \in V_+}\left\{\bar{q}_u^{\mathrm{C}}\right\}\right\},$$
$$\bar{q}_{h_i}^{\mathrm{C}} = \max\left\{0, q_{h_i}^{\mathrm{C}} - \varepsilon\right\}, \quad \bar{q}_{v_i}^{\mathrm{C}} = \max\left\{0, q_{v_i}^{\mathrm{C}} - n\varepsilon\right\}, \quad i \in \{1, \ldots, n\}.$$

We now check the feasibility of $\bar{q}^{\mathrm{C}}$. To this end, we first verify that $\bar{q}^{\mathrm{C}}$ satisfies Conditions (3). Conditions (3a) are satisfied due to $\bar{q}_s^{\mathrm{C}} \geq \bar{q}_u^{\mathrm{C}}$ for $u \in V_+$. We next show that Conditions (3b) hold. To this end, we distinguish between two cases.

First, assume $q_w^{\mathrm{C}} \leq n\varepsilon$ for all $w \in V_-$. Consequently, $\bar{q}_s^{\mathrm{C}} = \max\left\{\bar{q}_u^{\mathrm{C}} : u \in V_+\right\}$ and $\bar{q}_{v_i}^{\mathrm{C}} = 0$ for $i \in \{1, \ldots, n\}$ are satisfied, which implies Conditions (3b). Second, assume there exists $v \in V_-$ with $q_v^{\mathrm{C}} > n\varepsilon$. If additionally

$$\max\left\{\bar{q}_w^{\mathrm{C}} : w \in V_-\right\} = \max\left\{\bar{q}_u^{\mathrm{C}} : u \in V_+\right\} = \bar{q}_s^{\mathrm{C}}$$

holds, then Conditions (3b) directly follow. Otherwise, from the feasibility of q^{C} and the construction of $\bar{q}^{\mathrm{C}}$,

$$\sum_{u \in V_+} \bar{q}_u^{\mathrm{C}} \geq \sum_{u \in V_+} q_u^{\mathrm{C}} - n\varepsilon \geq \max_{w \in V_-} q_w^{\mathrm{C}} - n\varepsilon = \max_{w \in V_-} \bar{q}_w^{\mathrm{C}}$$

follows, which implies (3b). Thus, Conditions (3) are satisfied by $\bar{q}^{\mathrm{C}}$. For checking the feasibility of $\bar{q}^{\mathrm{C}}$, it is left to show that Conditions (11) are satisfied for $\bar{q}^{\mathrm{C}}$. Due to the optimality of q^{C}, we can apply Lemma 3.11 and, thus, $q_{h_i}^{\mathrm{C}} \leq Z_i$ for $i \in \{1, \ldots, n\}$. Due to this and the construction of $\bar{q}^{\mathrm{C}}$, Conditions (11a) are satisfied. Thus, $\bar{q}_t^{\mathrm{C}} \leq \delta$ as well as Conditions (11c) and (11e) are satisfied. We next show that (11d) holds for $\bar{q}^{\mathrm{C}}$. The construction of $\bar{q}^{\mathrm{C}}$ and $q_{h_i}^{\mathrm{C}} \leq Z_i \leq M$ for $i \in \{1, \ldots, n\}$ leads to

$$\sum_{u \in V_+ \setminus \{t\}} \bar{q}_u^{\mathrm{C}} \leq \sum_{u \in V_+ \setminus \{t\}} q_u^{\mathrm{C}}, \quad \bar{q}_s^{\mathrm{C}} \leq \max\left\{q_s^{\mathrm{C}}, M\right\}.$$

This, together with the feasibility of Condition (11d) for q^{C}, leads to

$$0 \leq \min\left\{\sum_{u \in V_+ \setminus \{t\}} \bar{q}_u^{\mathrm{C}}, \bar{q}_s^{\mathrm{C}}\right\} \leq \min\left\{\sum_{u \in V_+ \setminus \{t\}} q_u^{\mathrm{C}}, \max\left\{q_s^{\mathrm{C}}, M\right\}\right\} \leq q_{(o,s)}^{+} = M,$$

which implies the feasibility of Condition (11d) for $\bar{q}^{\mathrm{C}}$. From Lemma 3.10, the construction of $\bar{q}^{\mathrm{C}}$, and the feasibility of q^{C} Condition (11f) follows.

We now show the feasibility of Condition (11b). For $i \in \{1, \ldots, n\}$, we prove

$$\sum_{u \in V_+ \setminus \{h_i\}} \bar{q}_u^{\mathrm{C}} = q_t^{\mathrm{C}} + \varepsilon + \sum_{u \in V_+ \setminus \{t, h_i\}} \max\left\{0, q_u^{\mathrm{C}} - \varepsilon\right\} \leq \max\left\{\sum_{u \in V_+ \setminus \{h_i\}} q_u^{\mathrm{C}}, \delta\right\}. \quad (14)$$

If $u \in V_+ \setminus \{t, h_i\}$ with $q_u^{\mathrm{C}} > \varepsilon$ does not exist, then

$$\sum_{u \in V_+ \setminus \{h_i\}} \bar{q}_u^{\mathrm{C}} = q_t^{\mathrm{C}} + \varepsilon \leq \delta$$

holds. Otherwise, an entry $w \in V_+ \setminus \{t, h_i\}$ with $q_w^{\mathrm{C}} > \varepsilon$ exists and

$$\sum_{u \in V_+ \setminus \{h_i\}} \bar{q}_u^{\mathrm{C}} = q_t^{\mathrm{C}} + \varepsilon + q_w^{\mathrm{C}} - \varepsilon + \sum_{u \in V_+ \setminus \{t, w, h_i\}} \bar{q}_u^{\mathrm{C}} \leq \sum_{u \in V_+ \setminus \{h_i\}} q_u^{\mathrm{C}}$$

is satisfied.

Using (14), the feasibility of q^{C}, and the construction of $\bar{q}^{\mathrm{C}}$, we show the feasibility w.r.t. Condition (11b) for $\bar{q}^{\mathrm{C}}$ by

$$\begin{aligned} 0 &\leq \min \left\{ \sum_{u \in V_+ \setminus \{h_i\}} \bar{q}_u^{\mathrm{C}}, \bar{q}_{v_i}^{\mathrm{C}} \right\} \\ &\leq \min \left\{ \max \left\{ \sum_{u \in V_+ \setminus \{h_i\}} q_u^{\mathrm{C}},\ \delta \right\}, q_{v_i}^{\mathrm{C}} \right\} \leq M + \delta - Z_i = q_{(o,h_i)}^{+}. \end{aligned}$$

Consequently, Conditions (11) are satisfied by $\bar{q}^{\mathrm{C}}$ and, thus, $\bar{q}^{\mathrm{C}}$ are feasible technical capacities due to Lemma 3.6.

Lastly, we compare the objective values of $\bar{q}^{\mathrm{C}}$ and q^{C} by

$$d^\top \bar{q}^{\mathrm{C}} - d^\top q^{\mathrm{C}} \geq \varepsilon d_t - \sum_{i=1}^{n} n\varepsilon d_{v_i} - n\varepsilon d_s \geq \varepsilon (d_t - n^2 - n d_s) = \varepsilon \geq 0.$$

Consequently, $\bar{q}^{\mathrm{C}}$ is a strictly better solution if $\varepsilon > 0$. □

In what follows, we show that the aggregated capacity of certain entries is bounded for optimal technical capacities in $G(\mathsf{SSP})$.

Lemma 3.13 *Let $q^C \in C$ be optimal technical capacities in $G(\mathsf{SSP})$. Then, $\sum_{u \in V_+ \setminus \{t\}} q_u^C \leq M$ is satisfied.*

Proof We prove the claim by contraposition. To this end, we assume that $\sum_{u \in V_+ \setminus \{t\}} q_u^{\mathrm{C}} > M$ holds. This together with Lemma 3.12 implies $q_t^{\mathrm{C}} = \delta$ and, hence,

$$\sum_{u \in V_+} q_u^{\mathrm{C}} > M + \delta. \tag{15}$$

By Lemma 3.6, the feasible technical capacities q^{C} satisfy Conditions (11). Because of the assumption, the inequality $q_s^{\mathrm{C}} \leq M$ follows from Condition (11d). Due to Lemma 3.11, $q_{h_i}^{\mathrm{C}} \leq Z_i$ for $i \in \{1, \ldots, n\}$. This, Inequality (15), and Condition (11b), imply $q_{v_i}^{\mathrm{C}} \leq M + \delta - Z_i$ for $i \in \{1, \ldots, n\}$.

We now bound the objective value of q^{C} by

$$d^\top q^{\mathrm{C}} \leq \sum_{i=1}^{n} (M + \delta - Z_i) - M + M d_s + d_t \delta = T - d_s \delta - M.$$

Thus, from Lemma 3.8 it follows that q^{C} is not optimal. □

With the next two lemmas, we bound the objective value of the ith branch of $G(\mathrm{SSP})$ in optimal technical capacities depending on the amount of flow, which is supplied to this branch. In doing so, the ith branch consists of the subtree that includes the nodes o, h_i, and v_i.

Lemma 3.14 *Let $q^C \in C$ be optimal technical capacities and $i \in \{1, \ldots, n\}$. If $\sum_{u \in V_+ \setminus \{h_i\}} q_u^C > M + \delta - Z_i$ holds, then*

$$q_{v_i}^C = M + \delta - Z_i, \quad d_{h_i} q_{h_i}^C + d_{v_i} q_{v_i}^C = -q_{h_i}^C + M + \delta - Z_i$$

holds.

Proof Let $q^C \in C$ be optimal technical capacities and $i \in \{1, \ldots, n\}$. Due to $\sum_{u \in V_+ \setminus \{h_i\}} q_u^C > M + \delta - Z_i$ and the feasibility of q^C, it follows from Conditions (11b) that q^C is only feasible if $q_{v_i}^C \leq M + \delta - Z_i$ holds. Using this, $Z_i \leq M + \delta$, the optimality of q^C, $d_{v_i} > 0$, Lemmas 3.10–3.12, and Conditions (11) leads to $q_{v_i}^C = M + \delta - Z_i$, which shows the claim. □

Lemma 3.15 *Let $q^C \in C$ be optimal technical capacities and $i \in \{1, \ldots, n\}$. If $\sum_{u \in V_+ \setminus \{h_i\}} q_u^C \leq M + \delta - Z_i$ holds, then*

$$q_{v_i}^C = \sum_{u \in V_+} q_u^C, \quad d_{h_i} q_{h_i}^C + d_{v_i} q_{v_i}^C = -q_{h_i}^C + \sum_{u \in V_+} q_u^C$$

holds.

Proof Let $q^C \in C$ be optimal technical capacities, which satisfy the requirements and $i \in \{1, \ldots, n\}$. Due to Conditions (3b), the inequality $q_{v_i}^C \leq \sum_{u \in V_+} q_u^C$ is satisfied. For any assignment $q_{v_i}^C \in [0, \sum_{u \in V_+} q_u^C]$, the Conditions (11) are satisfied by q^C due to $\sum_{u \in V_+ \setminus \{h_i\}} q_u^C \leq M + \delta - Z_i$ and Lemmas 3.10–3.12. Thus, the optimality of q^C, and $d_{v_i} > 0$, $q_{v_i}^C = \sum_{u \in V_+} q_u^C$ holds and the claim follows. □

We now derive an upper bound for the objective value if the given SSP instance is infeasible while the aggregated entry capacity is $M + q_t^C$.

Lemma 3.16 *Let the given SSP be infeasible, i.e., there exists no subset $I \subseteq \{1, \ldots, n\}$ with $\sum_{i \in I} Z_i = M$. Let $q^C \in C$ be optimal technical capacities in $G(\mathrm{SSP})$ with $\sum_{u \in V_+ \setminus \{t\}} q_u^C = M$. Then, $d^\top q^C < T$ holds.*

Proof Due to Lemma 3.12, $q_t^C = \delta$ holds. Consequently, $\sum_{u \in V_+} q_u^C = M + \delta$ is satisfied. We now compute an upper bound for the ith branch (12) in $G(\mathrm{SSP})$ depending on $i \in \{1, \ldots, n\}$. Due to Lemma 3.11, $q_{h_i}^C \leq Z_i$ holds.

If $q_{h_i}^C < Z_i$ holds, then

$$\sum_{u \in V_+ \setminus \{h_i\}} q_u^C = M + \delta - q_{h_i}^C > M + \delta - Z_i.$$

Hence, we apply Lemma 3.14, and thus, (12) evaluates to $-q_{h_i}^C + M + \delta - Z_i$. If $q_{h_i}^C = Z_i$ holds, then

$$\sum_{u \in V_+ \setminus \{h_i\}} q_u^C = M + \delta - q_{h_i}^C = M + \delta - Z_i.$$

Consequently, we can apply Lemma 3.15 and, thus, (12) evaluates to $M + \delta - Z_i$. From Lemma 3.11, it follows $q^{\mathrm{C}}_{h_i} \in [0, Z_i]$ for $i \in \{1, \dots, n\}$. Due to this, the infeasibility of SSP, $q^{\mathrm{C}}_t = \delta$, and $\sum_{u \in V_+ \setminus \{t\}} q^{\mathrm{C}}_u = M$, an index $j \in \{1, \dots, n\}$ exists with $q^{\mathrm{C}}_{h_j} \in (0, Z_j)$. Also using Lemma 3.10, we can bound the objective value of q^{C} by

$$\begin{aligned} d^\top q^{\mathrm{C}} &\leq \sum_{i=1, i \neq j}^{n} (M + \delta - Z_i) + (M + \delta - Z_j - q^{\mathrm{C}}_{h_j}) + d_s(M + \delta) + d_t \delta \\ &< \sum_{i=1}^{n} (M + \delta - Z_i) + d_s(M + \delta) + d_t \delta = T. \end{aligned}$$ □

We now prove an upper bound for the objective value of optimal technical capacities independent of the SSP being feasible while the aggregated entry capacity is below $M + q^{\mathrm{C}}_t$.

Lemma 3.17 *Let $q^C \in C$ be optimal technical capacities in $G(SSP)$ and $\sum_{u \in V_+ \setminus \{t\}} q^C_u = M - \varepsilon$ for a fixed $\varepsilon \in (0, M]$. Then, $d^\top q^C < T$ holds.*

Proof Due to Lemma 3.12, $q^{\mathrm{C}}_t = \delta$ holds, which implies $\sum_{u \in V_+} q^{\mathrm{C}}_u = M + \delta - \varepsilon$. We now compute an upper bound for the ith branch (12) of $G(\mathrm{SSP})$ depending on $i \in \{1, \dots, n\}$. Let $i \in \{1, \dots, n\}$. If $q^{\mathrm{C}}_{h_i} < Z_i - \varepsilon$ holds, then

$$\sum_{u \in V_+ \setminus \{h_i\}} q^{\mathrm{C}}_u = M + \delta - \varepsilon - q^{\mathrm{C}}_{h_i} > M + \delta - Z_i.$$

We apply Lemma 3.14 and, thus, the ith branch (12) evaluates to $-q^{\mathrm{C}}_{h_i} + M + \delta - Z_i$. If, on the other hand, $q^{\mathrm{C}}_{h_i} \geq Z_i - \varepsilon$ holds, then

$$\sum_{u \in V_+ \setminus \{h_i\}} q^{\mathrm{C}}_u = M + \delta - \varepsilon - q^{\mathrm{C}}_{h_i} \leq M + \delta - Z_i.$$

We now apply Lemma 3.15, which together with $q^{\mathrm{C}}_{h_i} \geq Z_i - \varepsilon$, Conditions (3), and the requirements implies that the objective of the ith branch (12) is bounded by

$$-q^{\mathrm{C}}_{h_i} + q^{\mathrm{C}}_{v_i} \leq -q^{\mathrm{C}}_{h_i} + (M + \delta - \varepsilon) \leq M + \delta - Z_i.$$

From $\sum_{u \in V_+} q^{\mathrm{C}}_u = M + \delta - \varepsilon$ and Condition (3b), it follows $q^{\mathrm{C}}_s \leq M + \delta - \varepsilon$. Due to this and the above, we can bound the objective value of q^{C} from above by

$$d^\top q^{\mathrm{C}} \leq \sum_{i=1}^{n} (M + \delta - Z_i) + d_s(M + \delta - \varepsilon) + d_t \delta = T - d_s \varepsilon < T.$$ □

The next theorem describes the relation between deciding the feasibility of a given SSP instance and computing optimal technical capacities in $G(\mathrm{SSP})$.

Lemma 3.18 *The SSP problem is solvable if and only if the optimal technical capacities $q^C \in C$ in $G(SSP)$ satisfy*

$$d^\top q^C \geq T. \tag{16}$$

Proof Let the SSP problem be solvable and q^{C} be optimal technical capacities in $G(\mathsf{SSP})$. We apply Lemma 3.9 and, thus, (16) is satisfied.

Let now $q^{\mathrm{C}} \in C$ be optimal technical capacities in $G(\mathsf{SSP})$ that satisfy (16). We now assume that SSP is infeasible. Due to the optimality of q^{C} and Lemma 3.13, we know that $\sum_{u \in V_+ \setminus \{t\}} q_u^{\mathrm{C}} \leq M$ holds. If $\sum_{u \in V_+ \setminus \{t\}} q_u^{\mathrm{C}} = M$ holds, then we apply Lemma 3.16, which is a contradiction to q^{C} satisfying (16). If $\sum_{u \in V_+ \setminus \{t\}} q_u^{\mathrm{C}} = M - \varepsilon$ for a fixed $\varepsilon \in (0, M]$ holds, we apply Lemma 3.17, which is a contradiction to q^{C} satisfying (16). □

We finally prove that CTC is NP-complete on trees.

Theorem 3.19 *CTC with capacitated linear flows is NP-*complete *on trees. On general graphs, it is at least NP-*hard.

Proof The feasibility of given technical capacities can be verified in polynomial time on trees; see Theorem 3.7.

For a given SSP instance, we can construct the CTC instance $G(\mathsf{SSP})$ in polynomial time and its coding length is polynomially bounded above by the coding length of the given SSP instance. Hence, from Lemma 3.18 it follows that CTC is NP-hard on trees, since $G(\mathsf{SSP})$ is a tree. □

4 Computing technical capacities for nonlinear potential-based flows

We now consider a nonlinear potential-based flow model of gas transport. Thus, the flows depend on the potentials at the incident nodes. In contrast to the capacitated linear flow case, the flows in potential-based networks follow additional physical laws that make it unique. On the one hand, the potentials provide additional structure for the analysis of nominations, bookings, and technical capacities. On the other hand, the coupling between potentials and flows is usually nonlinear, which results in a harder class of optimization problems. For capacitated linear flows it is shown that checking the feasibility of technical capacities, respectively bookings, is coNP-complete on general networks; see Hayn (2016). In Labbé et al. (2020), it is shown that verifying the feasibility of technical capacities, respectively bookings, can be solved in polynomial time on networks with linear potential-based flows. Moreover, checking the feasibility of technical capacities, respectively bookings, can be done in polynomial time on trees and single cycle networks in case of nonlinear potential-based flows; see Labbé et al. (2019, 2020). For the complexity of CTC with potential-based flows, only exponential upper complexity bounds are known so far; see Hayn (2016).

In this section, we prove that CTC is NP-complete for nonlinear as well as linear potential-based flows. We first prove this for the nonlinear potential-based case. Afterward, we show that the linear potential-based case can be proven in analogy with the help of minor adaptions.

We now explicitly state the considered nonlinear potential-based flow model. To this end, we introduce a bounded potential variable p_u for every node $u \in V$. Additionally, the potentials are coupled to arc flows. Thus, for a nomination $\ell \in N$ the Constraints (1) are given by (2) and the classical Weymouth pressure drop conditions

$$p_v^2 = p_u^2 - \Lambda_a |q_a| q_a \quad \text{for all } a = (u, v) \in A, \tag{17}$$

where $\Lambda_a > 0$ is a constant for every arc $a \in A$; see Weymouth (1912); Ríos-Mercado and Borraz-Sánchez (2015) and the chapter Fügenschuh et al. (2015) in the book Koch et al. (2015). Furthermore, the pressures are bounded, i.e.,

$$0 < p_u^- \le p_u \le p_u^+ \quad \text{for all } u \in V. \tag{18}$$

Consequently, the Constraints (1) are given by

$$c_{\mathcal{I}}^{\text{pot}}(x) = \left(c_{\mathcal{I},u}^{\text{pot}}(p)_{u\in V}\right) \quad \text{with} \quad c_{\mathcal{I},u}^{\text{pot}}(p) = (p_u - p_u^-, p_u^+ - p_u)$$

as well as

$$c_{\mathcal{E}}^{\text{pot}}(x;\ell) = \begin{pmatrix} (c_{\mathcal{E},u}^{\text{pot}}(q;\ell))_{u\in V} \\ (c_{\mathcal{E},a}^{\text{pot}}(q,p))_{a\in A} \end{pmatrix}$$

with

$$c_{\mathcal{E},u}^{\text{pot}}(q;\ell) = \sum_{a\in\delta^{\text{out}}(u)} q_a - \sum_{a\in\delta^{\text{in}}(u)} q_a - \sigma_u \ell_u, \quad c_{\mathcal{E},a}^{\text{pot}}(q,p) = p_u^2 - p_v^2 - \Lambda_a |q_a| q_a.$$

In contrast to the capacitated linear flow model, no arc flow bounds exist in the potential-based model. Instead, potential bounds are now included.

We can check the feasibility of technical capacities in tree-shaped networks with potential-based flows in polynomial time due to Labbé et al. (2020).

Lemma 4.1 *Let $q^C \in C$ be technical capacities in the tree $G = (V, A)$. Then, we can decide if q^C is feasible and satisfies Condition (3) in polynomial time. In particular, this implies that CTC with nonlinear potential-based flows on trees is in NP.*

Proof Conditions (3) can obviously be checked in polynomial time. The feasibility of q^C can be checked in $O(|V|^2)$ due to Theorem 20 in Labbé et al. (2020). □

We note that checking the feasibility of q^C in polynomial time also follows from adapting Theorem 4 in Robinius et al. (2019).

Considering a nonlinear potential-based flow model, we now prove that CTC is NP-hard in tree-shaped networks. To this end, we reduce CTC with capacitated linear flows to CTC with nonlinear potential-based flows. The case of capacitated linear flows is NP-hard due to the results of Sect. 3. Thus, we now focus on the reduction instances G(SSP) of the capacitated linear flow case; see Sect. 3.

We now transform a given G(SSP) instance of the capacitated linear flow to the potential-based case. To this end, we take the same graph $G(\text{SSP}) = (V, A)$ and the objective coefficients d as in the previous section. We remove the flow bounds. Moreover, we set $\Lambda_{(t,s)} = (M+\delta)^2 10^2 d_t^2$ and $\Lambda_a = 1$ for all remaining arcs $a \in A \setminus \{(t,s)\}$. The squared potential bounds are given in Table 2. Intuitively, $K = 2(M+\delta)$ is a pressure value that is chosen high enough such that the pressure never drops below zero in the network. We denote the constructed instance by G^{pot}(SSP). We further note that for a given instance of G(SSP), we can build G^{pot}(SSP) in polynomial time and its coding length is polynomially bounded above by the coding length of the given G(SSP) instance.

We first prove that feasible technical capacities in G(SSP) with capacitated linear flow are also feasible for G^{pot}(SSP) in the potential-based case.

Lemma 4.2 *Let $q^C \in C$ be feasible technical capacities in G(SSP) with capacitated linear flow. Then, q^C are feasible technical capacities in G^{pot}(SSP) in the potential-based model.*

Proof Since q^C are feasible technical capacities for G(SSP), they satisfy Conditions (3). Let $\ell \in N(q^C)$ be a nomination and q its corresponding flow, which is unique due to the tree structure of the underlying graph. We now prove that this nomination is also feasible in

Table 2 Squared potential bounds with $K = 2(M + \delta)$ and $\delta = (n+1)^{-1}$

Nodes	$(p^-)^2$	$(p^+)^2$
o	K	K
h_i	$K - (M + \delta - Z_i)^2$	$K + Z_i^2$
v_i	$K - (M + \delta - Z_i)^2 - (M + \delta)^2$	$K + Z_i^2$
s	$K - M^2$	$K + \delta^2$
t	$K - M^2$	$K + \delta^2 + \Lambda_{(t,s)}\delta^2$

$G^{\text{pot}}(\mathsf{SSP})$. To this end, we construct the potentials corresponding to q and $i \in \{1, \ldots, n\}$ as follows:

$$\begin{aligned} p_o^2 = K, \quad p_s^2 = K - |q_{(o,s)}|q_{(o,s)}, \quad p_t^2 = K - |q_{(o,s)}|q_{(o,s)} + \Lambda_{(t,s)}|q_{(t,s)}|q_{(t,s)}, \\ p_{h_i}^2 = K - |q_{(o,h_i)}|q_{(o,h_i)}, \quad p_{v_i}^2 = K - |q_{(o,h_i)}|q_{(o,h_i)} - |q_{(h_i,v_i)}|q_{(h_i,v_i)}. \end{aligned} \tag{19}$$

Since ℓ with its unique flows q is feasible for $G(\mathsf{SSP})$, they satisfy the flow bounds (10). Replacing the arc flows in (19) by the upper, respectively lower, arc flow bounds of $G(\mathsf{SSP})$, given by (10), shows that for any arc flows satisfying (10) the potentials given in (19) are within the lower and upper potential bounds of Table 2. Consequently, (q, p) satisfy Constraints (1) for the potential-based case and thus, ℓ is a feasible nomination for $G^{\text{pot}}(\mathsf{SSP})$. Since ℓ is an arbitrary booking-compliant nomination w.r.t. q^{C}, this shows the claim. □

We note that not all feasible technical capacities in $G^{\text{pot}}(\mathsf{SSP})$ for the potential-based case are also feasible in $G(\mathsf{SSP})$ with capacitated linear flow. For instance, technical feasible capacities with $q_t^{\mathrm{C}} > \delta$ exist that are feasible for $G^{\text{pot}}(\mathsf{SSP})$ but not for $G(\mathsf{SSP})$.

In contrast to feasible points, we now show that all optimal technical capacities in $G^{\text{pot}}(\mathsf{SSP})$ are also feasible in $G(\mathsf{SSP})$. To this end, we prove an upper bound for q_t^{C} and an analogous result to Lemma 3.11 for the potential-based case.

Lemma 4.3 *Let $q^C \in C$ be feasible technical capacities in $G^{pot}(SSP)$. Then, $q_t^C \le \delta + 1/(10 d_t)$ holds.*

Proof From Conditions (3), the squared potential bounds of Table 2, (17), and t being a leaf node of $G^{\text{pot}}(\mathsf{SSP})$, it follows

$$q_t^{\mathrm{C}} \le \sqrt{\delta^2 + \frac{1}{\Lambda_{(t,s)}}(\delta^2 + M^2)}.$$

Due to $\sqrt{a+b} \le \sqrt{a} + \sqrt{b}$ for $a, b \ge 0$ and the choice of $\Lambda_{(t,s)}$, we obtain

$$q_t^{\mathrm{C}} \le \sqrt{\delta^2 + \frac{1}{\Lambda_{(t,s)}}(\delta^2 + M^2)} \le \delta + \frac{1}{\sqrt{\Lambda_{(t,s)}}}(\delta + M) = \delta + \frac{1}{10 d_t}. \qquad \square$$

Lemma 4.4 *Let $q^C \in C$ be optimal technical capacities in $G^{pot}(SSP)$. Then, $q_{h_i}^C \le Z_i$ holds for all $i \in \{1, \ldots, n\}$.*

Proof We prove the claim by contraposition. Thus, we assume that $i \in \{1, \ldots, n\}$ with $q_{h_i}^{\mathrm{C}} > Z_i$ exists. From the tree structure of $G^{\text{pot}}(\mathsf{SSP})$, Lemmas 3.4 and 3.5, Conditions (3), and the potential bounds in Table 2, it follows that $\sum_{j=1, j\neq i}^{n} q_{v_j}^{\mathrm{C}} + q_s^{\mathrm{C}} \leq Z_i$. Thus, we obtain the bounds $q_s^{\mathrm{C}} \leq Z_i$, and $q_{v_j}^{\mathrm{C}} \leq Z_i$ for $j \in \{1, \ldots, n\} \setminus \{i\}$. Moreover, we obtain

$$q_{v_i}^{\mathrm{C}} \leq \sqrt{\frac{(p_{h_i}^{+})^2 - (p_{v_i}^{-})^2}{\Lambda_{(h_i, v_i)}}} = \sqrt{Z_i^2 + (M+\delta)^2 + (M+\delta-Z_i)^2} \leq 2(M+\delta).$$

Due to Lemma 4.3, $q_t^{\mathrm{C}} \leq \delta + 1/(10 d_t)$ holds. Furthermore, $d_{h_j} q_{h_j}^{\mathrm{C}} \leq 0$ holds for $j \in \{1, \ldots, n\} \setminus \{i\}$ and, thus, we can neglect these terms for bounding the objective value corresponding to q^{C} by

$$\begin{aligned} d^{\top} q^{\mathrm{C}} &\leq \left(\delta + \frac{1}{10 d_t}\right) d_t + Z_i d_s + (n-1) Z_i - Z_i + 2\,(M+\delta) \\ &\leq \left(\delta + \frac{1}{10 d_t}\right) d_t + Z_i d_s + nM + 2\delta. \end{aligned} \tag{20}$$

A comparison of the upper bound (20) for the objective value corresponding to q^{C} and the objective value of the feasible solution $\tilde{q}^{\mathrm{C}}$ in Lemma 3.8, which is also feasible for the potential-based case due to Lemma 4.2, leads to

$$\begin{aligned} &d^{\top} \tilde{q}^{\mathrm{C}} - d^{\top} q^{\mathrm{C}} \geq -\frac{1}{10 d_t} d_t + \delta d_s - M - nM - 2\delta \\ &= -\frac{1}{10} + (n+1)M + 1 - (n+1)M - \frac{2}{n+1} = 1 - \frac{1}{10} - \frac{2}{n+1} > 0 \end{aligned}$$

if $n \geq 2$. Hence, q^{C} is not optimal. □

We now prove that in an optimal solution q_t^{C} is bounded above by δ, which is also the case for the capacitated linear flow model; see Lemma 3.12.

Lemma 4.5 *Let $q^{\mathrm{C}} \in C$ be optimal technical capacities in $G^{pot}(SSP)$. Then, $q_t^{\mathrm{C}} \leq \delta$ holds.*

Proof We prove the claim by contraposition. Thus, we assume $q_t^{\mathrm{C}} > \delta$. Due to this, Lemmas 3.4 and 3.5, and the potential bounds in Table 2, it follows $\sum_{u \in V_- \setminus \{s\}} q_u^{\mathrm{C}} \leq \delta$. Consequently, $\sum_{u \in V_- \setminus \{s\}} d_u q_u^{\mathrm{C}} \leq \delta$ holds due to $d_u \leq 1$ for all $u \in V_- \setminus \{s\}$. Further, from the potential bounds, Lemma 4.3, and Conditions (3), the inequality $q_s^{\mathrm{C}} \leq M + \delta + 1/(10 d_t)$ follows. We now compare the objective value of q^{C} with the corresponding objective value of the solution $\tilde{q}^{\mathrm{C}}$ of Lemma 3.8.

First, assume that $q_s^{\mathrm{C}} \geq M + \delta$ holds. Due to Conditions (3) and $q_t^{\mathrm{C}} \leq \delta + 1/(10 d_t)$, which follows from Lemma 4.3, $\sum_{u \in V_+ \setminus \{t\}} q_u^{\mathrm{C}} \geq M - 1/(10 d_t) > 0$ holds. Consequently, a comparison of the objective values of q^{C} and $\tilde{q}^{\mathrm{C}}$ of Lemma 3.8 leads to

$$\begin{aligned} d^{\top} \tilde{q}^{\mathrm{C}} - d^{\top} q^{\mathrm{C}} &\geq -\frac{1}{10 d_t} d_t - \frac{1}{10 d_t} d_s - M - \sum_{u \in V_+ \setminus \{t\}} q_u^{\mathrm{C}} d_u - \sum_{u \in V_- \setminus \{s\}} q_u^{\mathrm{C}} d_u + n\delta \\ &\geq -\frac{1}{10 d_t} d_t - \frac{1}{10 d_t} d_s - M + \left(M - \frac{1}{10 d_t}\right) - \delta + n\delta \\ &\geq -\frac{3}{10} + (n-1)\delta > 0. \end{aligned}$$

Since $n \geq 2$ holds, q^{C} is not optimal. Second, assume that $q_s^{\mathrm{C}} < M + \delta$ holds. Thus, $\varepsilon > 0$ with $q_s^{\mathrm{C}} + \varepsilon = M + \delta$ exists. Due to Conditions (3) and $q_t^{\mathrm{C}} \leq \delta + 1/(10 d_t)$, which follows from Lemma 4.3, $\sum_{u \in V_+ \setminus \{t\}} q_u^C \geq \max\{0, M - \varepsilon - 1/(10d_t)\}$ holds. Consequently, a comparison of the objective values of q^C and $\tilde{q}^C$ of Lemma 3.8 leads to

$$d^\top \tilde{q}^C - d^\top q^C \geq -\frac{1}{10d_t} d_t + \varepsilon d_s - M + \max\left\{0, M - \varepsilon - \frac{1}{10d_t}\right\} - \delta + n\delta. \quad (21)$$

If $\max\{0, M - \varepsilon - 1/(10d_t)\} = 0$ is satisfied, then $\varepsilon \geq 0.9$ holds. Thus, (21) is positive for $n \geq 2$. Otherwise, (21) results in

$$-\frac{1}{10} + \varepsilon d_s - \varepsilon - \frac{1}{10d_t} - \delta + n\delta > 0.$$

Hence, q^C is not optimal. □

Lemma 4.6 *Let $q^C \in C$ be optimal technical capacities in $G^{pot}(SSP)$. Then, q^C are feasible technical capacities in $G(SSP)$.*

Proof Since q^C are feasible technical capacities for the potential-based case, they satisfy Conditions (3). We now check if q^C satisfies Conditions (11). Due to Lemma 4.4, $q_{h_i}^C \leq Z_i$ holds for all $i \in \{1, \ldots, n\}$. Consequently, Condition (11a) is satisfied. Due to Lemma 4.5, $q_t^C \leq \delta$ holds as well. Thus, Conditions (11c) and (11e) are satisfied. From Conditions (3), the potential bounds in Table 2, Lemmas 3.4 and 3.5, and $q_{h_i}^C \leq Z_i$, it follows $q_{v_i}^C \leq M + \delta$ for $i \in \{1, \ldots, n\}$. Consequently, Condition (11f) is satisfied.

The potential bounds in Table 2 imply that the flow on arc (o, s) is bounded from the above by M and the arc flow (o, h_i) is bounded from below by $-Z_i$ as well as from above by $M + \delta - Z_i$ for $i \in \{1, \ldots, n\}$. Due to this and Lemmas 3.4 and 3.5, Conditions (11d) and (11b) are satisfied. In total, q^C satisfies Conditions (11) and thus, the claim follows from Lemma 3.6. □

Lemma 4.7 *The optimal technical capacities in $G(SSP)$ and in $G^{pot}(SSP)$ are identical.*

Proof The claim follows from Lemmas 4.2 and 4.6. □

As a consequence of the last lemma, the Lemmas 3.10–3.17 are also valid in the potential-based case. Thus, we can also adapt Lemma 3.18, which implies that CTC on trees with a nonlinear potential-based model is NP-hard .

Lemma 4.8 *The SSP problem is solvable if and only if the optimal technical capacities q^C of $G^{pot}(SSP)$ satisfy $d^\top q^C \geq T$.*

Proof The claim follows from Lemmas 4.7 and 3.18. □

Theorem 4.9 *CTC with nonlinear potential-based flows is NP*-complete *on trees. On general graphs, it is at least NP*-hard .

Proof The validation of a given technical capacities of a tree can be done in polynomial time due to Lemma 4.1. Then, the claim follows from Lemma 4.8. □

Sometimes linear potential-based flow models are preferred instead of the nonlinear potential-based model here considered, since it simplifies the resulting optimization problem. The only difference between a linear and our nonlinear potential-based model is that the Weymouth equations (17) are replaced by

$$p_v = p_u - \Lambda_a q_a \quad \text{for all } a = (u, v) \in A. \quad (22)$$

The remaining Constraints (1) stay the same. We conclude this section with proving that CTC for linear potential-based flows is also NP-complete on trees. This can be shown in analogy to the nonlinear potential-based case considering only a few small adaption.

Theorem 4.10 *CTC with linear potential-based flows is NP-*complete *on trees. On general graphs, it is NP-*complete *as well.*

Proof (Sketch) Checking the feasibility of technical capacities with linear potential-based flows in a general graph can be done in polynomial time due to Theorem 12 in Labbé et al. (2020). Consequently, CTC with linear potential-based flow is in NP .

For proving NP -hardness, we adapt the previous results for the nonlinear potential-based case. We first replace the original value $\Lambda_{(t,s)} = (M+\delta)^2 10^2 d_t^2$ by $\Lambda_{(t,s)} = (M+\delta)10d_t$. In analogy, we replace in Table 2 every squared value by its non-squared value. Furthermore, Table 2 now represents the potential bounds p^- and p^+ instead of $(p^-)^2$ and $(p^+)^2$. Finally, we replace the terms $|q_a|q_a$ by q_a and p_u^2 by p_u in (19). After these modifications, we can prove Lemmas 4.2–4.8 for the linear potential-based case in analogy to the nonlinear case—keeping in mind that the potentials are now coupled by (22), which simplifies some of the calculations.

This implies that CTC for linear potential-based flows is NP-hard on general graphs. □

5 Conclusion

In this paper, we proved that computing maximal technical capacities in the European entry-exit gas market is NP-hard. To this end, we showed that the problem is NP-complete on trees for a capacitated linear flow model as well as for potential-based flows. We first reduced the Subset Sum problem to computing maximal technical capacities with capacitated linear flows on trees. Afterward, we used this result to reduce the case of capacitated linear flows to the case of potential-based flows. In contrast to the situation in the literature on the feasibility of bookings, our hardness results for CTC are already obtained for the easiest case, i.e., on tree-shaped networks and capacitated linear flow models as well as potential-based flows. Consequently, computing technical capacities is also hard for more general graph classes including trees, i.e., especially for general graphs. Another interesting question regarding the complexity of CTC is whether it is Σ_2^{P}-complete for capacitated linear or nonlinear potential-based flows.

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Article 8

Global optimization for the multilevel European gas market system with nonlinear flow models on trees

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Global optimization for the multilevel European gas market system with nonlinear flow models on trees

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Abstract
The European gas market is implemented as an entry-exit system, which aims to decouple transport and trading of gas. It has been modeled in the literature as a multilevel problem, which contains a nonlinear flow model of gas physics. Besides the multilevel structure and the nonlinear flow model, the computation of so-called technical capacities is another major challenge. These lead to nonlinear adjustable robust constraints that are computationally intractable in general. We provide techniques to equivalently reformulate these nonlinear adjustable constraints as finitely many convex constraints including integer variables in the case that the underlying network is tree-shaped. We further derive additional combinatorial constraints that significantly speed up the solution process. Using our results, we can recast the multilevel model as a single-level nonconvex mixed-integer nonlinear problem, which we then solve on a real-world network, namely the Greek gas network, to global optimality. Overall, this is the first time that the considered multilevel entry-exit system can be solved for a real-world sized network and a nonlinear flow model.

Keywords European entry-exit gas market · Multilevel optimization · Robust optimization · Mixed-integer nonlinear optimization · Nonlinear flows

Mathematics Subject Classification 90B10 · 90C26 · 90C35 · 90C90

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1 Introduction

The European gas market is organized as a so-called entry-exit system. This market structure was introduced as a result of the European gas market liberalization [7,8] with the main goal to decouple transport and trading of natural gas. To this end, the market system is split into multiple levels, in which the transmission system operator (TSO) and gas traders interact with each other. The traders *book* capacities at nodes in the network, typically for a longer time period, e.g., months. They then *nominate* every day the amount of gas they want to trade at this node. To determine the capacity that can be booked at a point, the TSO allocates *technical capacities* in advance. These technical capacities are the main tool to decouple the transport and trading of gas. To achieve this goal, the TSO has to guarantee that every nomination below these technical capacities—i.e., infinitely many balanced load flows—can be transported through the network. As a consequence, gas trading within these technical capacities is no longer explicitly restricted by the actual transport of gas. The advantage of this setup is that the traders can completely ignore the physical network and that they only have to know the technical capacities that have been announced by the TSO.

The main goal that the entry-exit-system is meant to achieve is the "effective separation of supply and production activities from network operations" [7]. On the other hand, the entry-exit-system has some obvious drawbacks. By decoupling the different steps it is expected that economic inefficiencies arise. It is, however, very difficult to quantify the welfare losses of this system, which is the goal of the multilevel model studied in this paper. From a mathematical point of view, the allocation of technical capacities leads to a highly challenging nonlinear adjustable robust problem, which is one of the major computational challenges of the entry-exit market organization. For a general overview about adjustable robust optimization, we refer to [1,36] and the references therein. We will show how one can overcome these mathematical difficulties to analyze an entry-exit-system for a tree-shaped network with a nonlinear gas flow model. A multilevel mathematical model of an entry-exit-system has been proposed in [14], where it is also shown that it can be reformulated as an equivalent bilevel model under suitable assumptions. In a stylized way, the considered entry-exit system can be described along four subsequent and interconnected levels. First, the TSO has to allocate technical capacities to all nodes of the network. Afterward, the TSO and the gas traders sign mid- to long-term booking contracts in which the traders buy node-specific capacity-rights for the maximal injection or withdrawal of gas. The sum of these bookings at every node of the network is bounded from above by the previously allocated technical capacities. On the day-ahead market, the traders then nominate the amount of gas that they feed in or withdraw under the condition that these amounts are below their booked quantities. Lastly, the TSO operates the network such that the requested amount of gas is transported through the network.

The model in [14] does not prescribe the physical model underlying the gas flow. For simplified linear flow models, this model can be solved on stylized small and passive (but cyclic) networks, i.e., networks without active elements such as compressor stations or (control) valves; see [2]. Unfortunately, the techniques exploited in [2] cannot be applied to nonlinear flow models. In this paper, we focus on solving the multilevel problem for a nonlinear flow model. Since switching from a linear to a nonlinear flow model makes the computation of technical capacities much more challenging, we need to restrict ourselves to only considering tree-shaped networks. Our results allow for the first time to solve a multilevel entry-exit gas market model in a real-world sized network, namely a passive version of the Greek gas network.

Since even linear multilevel problems are highly challenging in general, see [17,20], and since we additionally consider nonlinear flow models on top of the multilevel structure, we need to make the following assumptions. First, the considered multilevel market model in [14] is based on the assumption of perfect competition among gas traders. Including strategic interaction is out of scope of this paper since strategic interaction alone leads to computationally challenging models in this context; see, e.g., [13]. Second, many different approaches exist for modeling gas physics. For a comprehensive overview see, e.g., the book [26] and the survey article [28] as well as the many references therein. We assume that our gas flow model represents a stationary potential-based flow and that the network does not contain active elements such as compressor stations or control valves. These assumptions allow us to consider the classic Weymouth equation for gas flows, which we formally introduce in Sect. 2. However, our findings hold for any nonlinear potential-based flow model under mild assumptions.

Let us note that the choice of modeling the gas physics directly influences the computational complexity of computing technical capacities, bookings, and nominations. For capacitated linear and linear potential-based flows, deciding the feasibility of a nomination is in P; see [5,19,24]. However, it is NP-hard in case of active elements; see [34]. Deciding the feasibility of a booking can be done in polynomial time for linear potential-based flows as well as in tree-shaped and single-cycle networks in case of nonlinear potential-based flows; see [21,22,29]. On the contrary, it is coNP-complete for capacitated linear flows, see [19], and it is coNP-hard for nonlinear potential-based flows; see [35]. In [32], structural properties such as (non-)convexity regarding the sets of feasible nominations and bookings are proven w.r.t. different models of gas transport. Finally, the computation of maximal technical capacities is NP-hard for capacitated linear and nonlinear potential-based flows even on trees; see [31]. Consequently, solving the considered multilevel entry-exit model including nonlinear flows poses a big challenge.

Our contribution is the following. We use the bilevel reformulation of the multilevel entry-exit gas market model presented in [14] and derive, as in [2], an exact single-level reformulation. In contrast to [2], we consider a nonlinear flow model of gas transport. The obtained single-level reformulation is still computationally intractable since it contains infinitely many nonlinear adjustable robust constraints that model technical capacities. We then derive for these constraints an equivalent finite-dimensional reformulation for the case of tree-shaped networks. This reformulation provides nice properties such that it consists of finitely many convex constraints including newly introduced integer variables. We further derive additional combinatorial constraints using the tree-shaped network structure that significantly speed up the solution process. Overall, we obtain a finite-dimensional nonconvex mixed-integer nonlinear single-level reformulation of the multilevel entry-exit gas market system. We then apply our results to solve the entry-exit model for a real-world network, namely the Greek gas network without active elements, to global optimality. Our computational results demonstrate the effectiveness of our techniques since the majority of the instances can be solved within 1 h. We further show that the additional combinatorial constraints are of great importance to achieve these short running times.

The remainder of this paper is structured as follows. In Sect. 2, we review the multilevel model and its bilevel reformulation as given in [14]. We then present the single-level reformulation in line with [2] and derive further model improvements in Sect. 3. Afterward, we handle the nonlinear adjustable robust constraints regarding the technical capacities in tree-shaped networks; see Sect. 4. In Sect. 5, we derive additional combinatorial constraints for the computation of technical capacities that significantly speed up the solution process.

Finally, we apply our findings to solve the entry-exit model for the real-world Greek gas network without active elements in Sect. 6.

2 A multilevel model of the entry-exit gas market system

In this section, we briefly review the optimization model of the European entry-exit gas market developed in [14]. Its structure is given by the European directive [7] and the subsequent regulation [8] as a result of the European market liberalization. As in [14], we informally describe the four decision steps that correspond to the timing of the considered entry-exit market. We then go into more detail for the bilevel model that is the basis for our further investigations. The four steps of the entry-exit gas market system can be briefly outlined as follows:

(i) Allocation of technical capacities and specification of booking price floors by the TSO.
(ii) Booking of capacity rights by gas traders.
(iii) Nomination of gas within the booked capacities by gas traders at the day-ahead market.
(iv) Transport of the nominations by the TSO at minimum costs.

In Section 3 of [14], it is shown that the gas market model can be formulated as a bilevel model. The upper level (4) represents the first and fourth step, in which the TSO takes action. The lower level (5) corresponds to the second and third step, in which the gas traders interact with each other. We note that for this model, the assumption of perfect competition is essential. Otherwise, combining step 2 and 3 leads to a multi-leader multi-follower game, which can be modeled as an equilibrium problem with equilibrium constraints; see, e.g., the recent paper [13] in which the strategic setting is studied in detail. A visualization of this bilevel reformulation is given in Figure 3 of [14].

In the following, we discuss the notation and motivate the objective functions and constraints of the bilevel model.

We first introduce some basic notation regarding the considered gas networks. We model a gas network as a directed and weakly connected graph $G = (V, A)$ with nodes V and arcs A. The set of nodes is partitioned into the set of entry nodes V_+, at which gas is injected, the set of exit nodes V_-, at which gas is withdrawn, and the remaining inner nodes V_0. We note that the model allows for multiple gas traders i at any single node of the network, i.e., $i \in \mathcal{P}_u$ for $u \in V_+ \cup V_-$. Moreover, we consider multiple time periods $t \in T$ of gas trading and transport with $|T| < \infty$. Due to the general hardness of the multilevel model, we consider stationary gas flow without active, i.e., controllable, elements such as valves or compressors. In the upper level (4), the TSO allocates technical capacities q^{TC}, specifies booking price floors $\underline{\pi}^{\text{book}}$, and is responsible to transport the gas in accordance with the nominations to maximize the total social welfare in the considered market. The decision variables of the first level are the technical capacities q^{TC}, the booking price floors $\underline{\pi}^{\text{book}}$, and the pressure and flow variables (p and q, respectively) to express the state of the network for each time period $t \in T$. Throughout this paper, we consider the optimistic notion of bilevel optimization. Thus, the leader also optimizes over the optimal solutions of the lower-level problem, which makes the bookings q^{book} and the nominations q^{nom} variables of the upper-level problem as well.

The objective function (4a) represents the total social welfare aggregated over the considered time periods T. Further, c_i^{var} are the variable production costs of a gas seller $i \in \mathcal{P}_u$ at node $u \in V_+$. For a gas buyer $i \in \mathcal{P}_u$ at node $u \in V_-$, elastic demand is modeled by the inverse demand function $P_{i,t}$. This function models the marginal price tolerance as a function of the demand. Using inverse demand functions is standard in such micro-economic settings; see, e.g., the seminal textbook [23]. There it is also justified that these functions $P_{i,t}$ are continuous and strictly decreasing, which we assume in the following for all $i \in \mathcal{P}_u$, $u \in V_-$, and $t \in T$. We discuss the transportation costs after we have introduced the physical modeling of the gas transport.

Next, we discuss the core regulatory constraint. Constraint (4d) ensures that all balanced nominations that comply with the technical capacities, i.e.,

$$\mathcal{N}(q^{\mathrm{TC}}) := \left\{ q^{\mathrm{nom}} \in \mathbb{R}^{V_+ \cup V_-} \,:\, 0 \leq q^{\mathrm{nom}} \leq q^{\mathrm{TC}}, \sum_{u \in V_+} q_u^{\mathrm{nom}} = \sum_{u \in V_-} q_u^{\mathrm{nom}} \right\},$$

can be transported through the considered network. This is formalized by $\mathcal{F}(\hat{q}^{\mathrm{nom}})$, which consists of the feasible transport solutions for $\hat{q}^{\mathrm{nom}}$. Many different approaches for modeling the set $\mathcal{F}(q^{\mathrm{nom}})$ exist. As mentioned earlier, we consider stationary gas flow without active elements such as (control) valves or compressor stations. We further focus on a nonlinear gas transport model that is based on the Weymouth pressure loss equation. Note that our results also hold for the general case of nonlinear potential-based flows, which we further explain in Remark 2.1.

For every node $u \in V$ of the gas network and time period $t \in T$, we denote the pressure level at node u by $p_{u,t}$ with corresponding bounds

$$0 < p_u^- \leq p_{u,t} \leq p_u^+ < \infty. \tag{1}$$

We further denote the flow on arc $a \in A$ by $q_{a,t}$. Note that arc flow $q_{a,t}$ can be negative if it flows in the opposite direction w.r.t. the orientation of the arc. For every time period $t \in T$, the flows have to satisfy flow conservation at every node of the network, which is modeled by

$$\begin{aligned}
\sum_{a \in \delta^{\mathrm{out}}(u)} q_{a,t} - \sum_{a \in \delta^{\mathrm{in}}(u)} q_{a,t} &= \sum_{i \in \mathcal{P}_u} q_{u,t}^{\mathrm{nom}}, && u \in V_+,\ t \in T,\\
\sum_{a \in \delta^{\mathrm{out}}(u)} q_{a,t} - \sum_{a \in \delta^{\mathrm{in}}(u)} q_{a,t} &= -\sum_{i \in \mathcal{P}_u} q_{u,t}^{\mathrm{nom}}, && u \in V_-,\ t \in T,\\
\sum_{a \in \delta^{\mathrm{out}}(u)} q_{a,t} - \sum_{a \in \delta^{\mathrm{in}}(u)} q_{a,t} &= 0, && u \in V_0,\ t \in T.
\end{aligned} \tag{2}$$

Here, $\delta^{\mathrm{out}}(u)$ represents the set of outgoing arcs and $\delta^{\mathrm{in}}(u)$ the set of incoming arcs at node u. We note that we need to impose different signs for the nominations of entries V_+ and exits V_- in (2) to model that gas is injected or withdrawn since a nomination is a nonnegative vector. For an arc $a \in A$ and a time period $t \in T$, the corresponding flow $q_{a,t}$ links the pressure levels at the incident nodes of arc a. This link is given by the following Weymouth-like pressure loss law

$$p_{u,t}^2 - p_{v,t}^2 = \Lambda_a q_{a,t} \left| q_{a,t} \right|, \quad a = (u, v) \in A,\ t \in T, \tag{3}$$

where $\Lambda_a > 0$ is an arc specific constant.

We finally turn to the modeling of the transportation costs c_t for $t \in T$. Here, we model transportation costs as proposed in [2]. As in the latter paper, we consider a passive network without active elements. However, the majority of transportation costs consist of the operating costs of active elements such as compressors. Usually, these transportation costs are driven by the pressure losses in the network. In order to mimic cost-optimal transport in a passive network, the costs are given by the absolute squared pressure losses in the entire network

$$\sum_{t \in T} c_t(p, q; q^{\text{nom}}) = \sum_{t \in T} \sum_{a=(u,v)} c_t^{\text{trans}} \left| p_{u,t}^2 - p_{v,t}^2 \right|,$$

where $c_t^{\text{trans}} > 0$ holds for $t \in T$. We note that using Constraints (3), we can equivalently reformulate the transport costs as follows:

$$\sum_{t \in T} c_t(p, q; q^{\text{nom}}) = \sum_{t \in T} \sum_{a=(u,v)} c_t^{\text{trans}} \left| p_{u,t}^2 - p_{v,t}^2 \right| = \sum_{t \in T} \sum_{a=(u,v)} c_t^{\text{trans}} \Lambda_a q_{a,t}^2.$$

The transportation costs also appear in Constraint (4c). This constraint ensures that the booking price floors are chosen such that they recover transportation costs and additional investment costs C. Finally, the coupling between the upper and lower level is expressed in Constraint (4f).

In the lower level (5), gas traders buy capacity rights, so-called bookings q^{book}, that determine the maximum amount of gas that can be nominated. All traders then nominate their individual load of gas that is only bounded above by the chosen booking. The goal of every trader is to maximize its own profit, i.e., the trader books a capacity right that later leads to a surplus maximizing nomination. In doing so, the traders are only restricted by the technical capacities and booking price floors determined by the TSO in the first level. Note that the gas buyers and sellers do not take into account flow balance equations as well as any other physical or technical restrictions of the transport network. This is a defining aspect of the entry-exit system. It is touted as one of its features that buyers and sellers of gas do not have to care about the state of the network when making their trading decisions—except for the bookings that limit the nominations.

The interplay of booking and nominating can be modeled as a multi-leader multi-follower game. This game is difficult to analyze (see [13]) and, hence, is not usable in our context. Under a number of assumptions (as discussed in [14]), however, the solution of the game can be expressed as the solution of an optimization problem. We use the strongest assumption considered in [14], i.e., we assume perfect competition both in the booking and the nomination process on the day-ahead markets for both buyers and sellers. This allows to rewrite both the model of the booking and the day-ahead markets as mixed nonlinear complementarity problems (MNCP). These MNCPs are equivalent to optimization problems and can then be aggregated into a single optimization problem.

The single optimization problem can be interpreted as follows: The objective (5a) maximizes the welfare of all traders, that is, the surplus of the buyers minus the generation costs of the sellers, and minus the booking costs of all traders. The constraints make sure that bookings stay within the technical capacities (5b), nominations stay within the bookings (5c), and that all nominations are balanced (5d).

In summary, we obtain the bilevel model

$$\max_{\substack{q^{\text{TC}}, \underline{\pi}^{\text{book}}, p, q, \\ q^{\text{book}}, q^{\text{nom}}}} \varphi(q^{\text{nom}}, p) = \sum_{t \in T} \left(\sum_{u \in V_-} \sum_{i \in \mathcal{P}_u} \int_0^{q_{i,t}^{\text{nom}}} P_{i,t}(s) \mathrm{d}s - \sum_{u \in V_+} \sum_{i \in \mathcal{P}_u} c_i^{\text{var}} q_{i,t}^{\text{nom}} \right) \tag{4a}$$

$$- \sum_{t \in T} \sum_{a=(u,v) \in A} c_t^{\text{trans}} \left| p_{u,t}^2 - p_{v,t}^2 \right| - C$$

$$\text{s.t.} \quad 0 \le q_u^{\text{TC}}, \ 0 \le \underline{\pi}_u^{\text{book}}, \qquad u \in V_+ \cup V_-, \tag{4b}$$

$$\sum_{u \in V_+ \cup V_-} \sum_{i \in \mathcal{P}_u} \underline{\pi}_u^{\mathrm{book}} q_i^{\mathrm{book}} = \sum_{t \in T} \sum_{a=(u,v) \in A} c_t^{\mathrm{trans}} \left| p_{u,t}^2 - p_{v,t}^2 \right| + C, \tag{4c}$$

$$\forall \hat{q}^{\mathrm{nom}} \in \mathcal{N}(q^{\mathrm{TC}}) : \mathcal{F}(\hat{q}^{\mathrm{nom}}) \neq \emptyset, \tag{4d}$$

$$(p, q) \in \mathcal{F}(q^{\mathrm{nom}}), \text{ i.e., } (p, q) \text{ satisfies (1)–(3)}, \tag{4e}$$

$$(q^{\mathrm{book}}, q^{\mathrm{nom}}) \in \arg\max (5), \tag{4f}$$

where the lower level is given by

$$\max_{q^{\mathrm{book}}, q^{\mathrm{nom}}} \sum_{t \in T} \left(\sum_{u \in V_-} \sum_{i \in \mathcal{P}_u} \int_0^{q_{i,t}^{\mathrm{nom}}} P_{i,t}(s) \mathrm{d}s - \sum_{u \in V_+} \sum_{i \in \mathcal{P}_u} c_i^{\mathrm{var}} q_{i,t}^{\mathrm{nom}} \right) \tag{5a}$$

$$- \sum_{u \in V_+ \cup V_-} \sum_{i \in \mathcal{P}_u} \underline{\pi}_u^{\mathrm{book}} q_i^{\mathrm{book}}$$

$$\text{s.t.} \quad \sum_{i \in \mathcal{P}_u} q_i^{\mathrm{book}} \leq q_u^{\mathrm{TC}}, \quad u \in V_+ \cup V_-, \tag{5b}$$

$$0 \leq q_{i,t}^{\mathrm{nom}} \leq q_i^{\mathrm{book}}, \quad i \in \mathcal{P}_u, \ u \in V_+ \cup V_-, \ t \in T, \tag{5c}$$

$$\sum_{u \in V_-} \sum_{i \in \mathcal{P}_u} q_{i,t}^{\mathrm{nom}} - \sum_{u \in V_+} \sum_{i \in \mathcal{P}_u} q_{i,t}^{\mathrm{nom}} = 0, \quad t \in T. \tag{5d}$$

In general, bilevel problems are nonconvex. Further, they are strongly NP-hard even in case of linear bilevel problems; see [17,20]. In addition, the upper level of the considered problem is very challenging itself as we briefly outline in the following. First, the upper level contains nonsmooth terms in the objective function, which also appear in (4c). Moreover, Constraint (4c) contains nonconvex bilinear terms $\underline{\pi}_u^{\mathrm{book}} q_i^{\mathrm{book}}$. Additionally, considering a nonlinear flow model for gas transport leads to nonconvex constraints in (4e). Finally, and most critical, (4d) is a nonlinear adjustable robust constraint, which, in general, is computationally intractable. From the point of view of robust optimization, Constraint (4d) is an adjustable robust constraint with uncertainty set $\mathcal{N}(q^{\mathrm{TC}})$. For a detailed explanation regarding the connection of computing technical capacities, respectively deciding the feasibility of a booking, and adjustable robustness, we refer to Remark 2.6 in [22]. For the considered nonlinear flow model, already deciding its feasibility is coNP-hard; see [35]. Due to the inherent difficulty of the problem, we focus on tree-shaped networks. This allows us to obtain a finite-dimensional reformulation of the nonlinear adjustable robust constraint (4d) in Sect. 4. Moreover, this reformulation has some nice properties such that it is a convex mixed-integer model.

Remark 2.1 We note that our results, especially the computation of the technical capacities in Sect. 4, are also valid for the general case of potential-based flows. This means that we can generally replace Constraints (1) and (3) by the potential-based flow model

$$0 < \pi_u^- \leq \pi_{u,t} \leq \pi_u^+ < \infty, \qquad u \in V, \ t \in T,$$

$$\pi_{u,t} - \pi_{v,t} = \phi_a(q_{a,t}), \qquad a = (u, v) \in A, \ t \in T,$$

where ϕ_a is a continuous, strictly increasing, and odd (i.e.,$\phi_a(-q_{a,t}) = -\phi_a(q_{a,t})$) function. The latter is rather natural in the context of utility networks. We note that the freedom of modeling ϕ_a is large and it ranges from simple linear models to sophisticated nonlinear ones. On the one hand, this allows to apply our results to many different gas transport models. In particular, this includes the case of non-horizontal pipes; see [26]. On the other hand, we can also apply our results to many other different network types such as water, hydrogen, or lossless DC power flow networks, if the physics is appropriately modeled; see [15].

In the next section, we reformulate the presented bilevel as a single-level problem and present further model improvements.

3 Reduction to a single level problem

Since the bilevel model (4) with lower level (5) contains nonlinearities in the upper and lower level and since the linking variables q^{TC} and $\underline{\pi}^{\mathrm{book}}$ are continuous, we replace the convex lower level by its necessary and sufficient first-order optimality conditions to obtain a single-level problem. This is in line with [2], where the multilevel problem is considered for a linear potential-based flow model. We can adapt the single-level reformulation of [2] since the lower level is independent of the considered gas flow model.

To obtain concave-quadratic upper- and lower-level objective functions w.r.t. the upper- or lower-level variables, we make the following assumption.

Assumption 1 All inverse market demand functions are linear and strictly decreasing, i.e., $P_{i,t}(q_{i,t}^{\mathrm{nom}}) = b_{i,t} q_{i,t}^{\mathrm{nom}} + a_{i,t}$ with $a_{i,t} > 0$ and $b_{i,t} < 0$ for all $i \in \mathcal{P}_u, u \in V_-, t \in T$.

This assumption is rather standard in multilevel modeling of energy markets; see, e.g., [2,11,12] and the many references therein. Since the lower-level (5) then is a concave-quadratic maximization problem with a linearly constrained feasible region, its KKT conditions are both necessary and sufficient; see, e.g., [3]. We now replace the lower level (5) by its KKT conditions, i.e., the stationarity conditions

$$-\underline{\pi}_u^{\mathrm{book}} - \beta_u + \sum_{t \in T} \gamma_{i,t}^{+} = 0, \qquad i \in \mathcal{P}_u,\ u \in V_+ \cup V_-, \tag{6a}$$

$$a_{i,t} + b_{i,t} q_{i,t}^{\mathrm{nom}} + \gamma_{i,t}^{-} - \gamma_{i,t}^{+} - \delta_t = 0, \qquad i \in \mathcal{P}_u,\ u \in V_-,\ t \in T, \tag{6b}$$

$$-c_i^{\mathrm{var}} + \gamma_{i,t}^{-} - \gamma_{i,t}^{+} + \delta_t = 0, \qquad i \in \mathcal{P}_u,\ u \in V_+,\ t \in T, \tag{6c}$$

primal feasibility (5b)–(5d), nonnegativity

$$\beta_u \geq 0, \qquad u \in V_+ \cup V_-, \tag{7a}$$

$$\gamma_{i,t}^{-}, \gamma_{i,t}^{+} \geq 0, \qquad i \in \mathcal{P}_u,\ u \in V_+ \cup V_-,\ t \in T, \tag{7b}$$

of inequality multipliers, and complementary slackness conditions

$$\beta_u \left(q_u^{\mathrm{TC}} - \sum_{i \in \mathcal{P}_u} q_i^{\mathrm{book}} \right) = 0, \qquad u \in V_+ \cup V_-, \tag{8a}$$

$$\gamma_{i,t}^{-} q_{i,t}^{\mathrm{nom}} = 0, \qquad i \in \mathcal{P}_u,\ u \in V_+ \cup V_-,\ t \in T, \tag{8b}$$

$$\gamma_{i,t}^{+} \left(q_i^{\mathrm{book}} - q_{i,t}^{\mathrm{nom}} \right) = 0, \qquad i \in \mathcal{P}_u,\ u \in V_+ \cup V_-,\ t \in T. \tag{8c}$$

Then, the bilevel problem (4) can be reformulated as the single-level problem

$$
\begin{aligned}
\max_{s} \quad & \varphi(q^{\mathrm{nom}}, p) && \text{(9a)}\\
\text{s.t.} \quad & \text{upper-level feasibility: (4b)–(4e)}, && \text{(9b)}\\
& \text{lower level: (5b)–(5d), (6)–(8)}, && \text{(9c)}
\end{aligned}
$$

where $s = (q^{\mathrm{TC}}, \underline{\pi}^{\mathrm{book}}, q^{\mathrm{book}}, q^{\mathrm{nom}}, p, q, \beta, \gamma^{-}, \gamma^{+}, \delta)$.[1]

3.1 Linearization of KKT complementarity conditions

Using the standard big-M method, see [9], we now linearize the nonconvex complementarity constraints (8). To this end, bounds for the primal and dual variables are necessary.

For the dual variables, we adopt the values of [2], which are independent from the chosen gas flow model. To this end, we introduce the following notation:

$$
\begin{aligned}
a_t^{\min} &:= \min\{a_{i,t} : i \in \mathcal{P}_u, u \in V_-\},\\
a_t^{\max} &:= \max\{a_{i,t} : i \in \mathcal{P}_u, u \in V_-\},\\
c_{\min}^{\mathrm{var}} &:= \min\{c_i^{\mathrm{var}} : i \in \mathcal{P}_u, u \in V_+\},\\
c_{\max}^{\mathrm{var}} &:= \max\{c_i^{\mathrm{var}} : i \in \mathcal{P}_u, u \in V_+\}.
\end{aligned}
$$

Furthermore, we need the following assumptions.

Assumption 2 For every $t \in T$, it holds $a_t^{\min} \geq c_{\min}^{\mathrm{var}}$ and $a_t^{\max} \geq c_{\max}^{\mathrm{var}}$.

The intuition behind this assumption is that every player can participate in the market in every time period: The gas buyer with smallest willingness to pay can still receive gas from the seller with the smallest variable costs. The assumption can be easily checked a priori. Furthermore, we assume that the network is designed in such a way that trading takes place in every time period.

Assumption 3 For every time period $t \in T$, there exists a node $u \in V_+ \cup V_-$ with $i \in \mathcal{P}_u$ so that $q_{i,t}^{\mathrm{nom}} > 0$ holds.

A violation of this assumption in reality would mean that there is no gas trading in the entire market at all for a certain time period. That this takes place is very unrealistic—thus, the assumption itself should always hold in practice.

For the following we use Lemmas 2–4 of [2], by which we obtain upper bounds for the booking price floors and bounds for the dual variables.

Lemma 3.1 ([2], Lemmas 2–4) *There exists an optimal solution of (9) with*

$$
\begin{aligned}
& 0 \leq \gamma_{i,t}^{-} \leq 2(a_t^{\max} - c_{\min}^{\mathrm{var}}), && i \in \mathcal{P}_u,\ u \in V_+ \cup V_-,\ t \in T, && \text{(10a)}\\
& 0 \leq \gamma_{i,t}^{+} \leq a_t^{\max} - c_{\min}^{\mathrm{var}}, && i \in \mathcal{P}_u,\ u \in V_+ \in V_-,\ t \in T, && \text{(10b)}\\
& 0 \leq \beta_u \leq \sum_{t \in T}(a_t^{\max} - c_{\min}^{\mathrm{var}}), && u \in V_+ \cup V_-, && \text{(10c)}\\
& \underline{\pi}_u^{\mathrm{book}} \leq \sum_{t \in T}(a_t^{\max} - c_{\min}^{\mathrm{var}}), && u \in V_+ \cup V_-. && \text{(10d)}
\end{aligned}
$$

[1] We note that in the specification of z all entries of the vector have to be transposed, but for ease of notation we do not carry this out and maintain this convention in the remainder of the paper.

We now provide bounds for certain primal variables of the bilevel problem (4), respectively its single-level reformulation (9). We further present additional feasible constraints that tighten these bounds. As previously mentioned, these bounds are necessary for the linearization of the complementarity conditions (8). To this end, we first prove properties regarding nominations, bookings, and technical capacities in an optimal solution, see Lemmas 3.2–3.4, that enable us to a priori bound the technical capacities; see Lemma 3.5.

From Lemma 3.1 and Corollary 1 in [2], we obtain that an optimal solution exists in which the booking of a player equals its maximum nomination.

Lemma 3.2 (Corollary 1 of [2]) *There exists an optimal solution of the bilevel problem (4) satisfying (10) and*

$$\max_{t \in T} \left\{ q_{i,t}^{\text{nom}} \right\} = q_i^{\text{book}} \tag{11}$$

for all $i \in \mathcal{P}_u$, $u \in V_+ \cup V_-$.

Using this result, we now prove that an optimal solution exists in which the bookings equal the technical capacities.

Lemma 3.3 *There exists an optimal solution of the bilevel problem (4) satisfying (10), (11), and*

$$q_u^{TC} = \sum_{i \in \mathcal{P}_u} q_i^{\text{book}} \tag{12}$$

for all $u \in V_+ \cup V_-$.

Proof From Lemma 3.2 it follows that a solution $z = (q^{\text{TC}}, \underline{\pi}^{\text{book}}, q^{\text{book}}, q^{\text{nom}}, p, q)$ of (4) satisfying (10) and (11) exists. We now set $\tilde{z} = (\tilde{q}^{\text{TC}}, \underline{\pi}^{\text{book}}, q^{\text{book}}, q^{\text{nom}}, p, q)$ with $\tilde{q}_u^{\text{TC}} = \sum_{i \in \mathcal{P}_u} q_i^{\text{book}}$ for $u \in V_+ \cup V_-$.

The feasible region of the lower level (5) w.r.t. z is a relaxation of the feasible region of (5) w.r.t. $\tilde{z}$ since

$$0 \leq \sum_{i \in \mathcal{P}_u} q_i^{\text{book}} = \tilde{q}_u^{\text{TC}} \leq q_u^{\text{TC}}, \quad u \in V_+ \cup V_-,$$

holds. However, due to the latter inequalities, $(q^{\text{book}}, q^{\text{nom}})$ is feasible for (5) w.r.t. $\tilde{z}$. We further note that the corresponding lower-level objective functions are equal. Consequently, the optimal solution $(q^{\text{book}}, q^{\text{nom}})$ of the lower-level (5) w.r.t. z is also optimal for (5) w.r.t. $\tilde{z}$.

Furthermore, $\tilde{z}$ satisfies the upper level constraints (4b)–(4f). We note that (4d) is valid due to $\hat{q}^{\text{nom}} \in \mathcal{N}(\tilde{q}^{\text{TC}}) \subseteq \mathcal{N}(q^{\text{TC}})$. Thus, $\tilde{z}$ is a bilevel feasible point of (4). Moreover, q^{TC} is not present in the upper-level objective function and hence, the optimal values corresponding to z and to $\tilde{z}$ are equal. Consequently, $\tilde{z}$ is an optimal solution of (4). □

Note that, despite the two last results, it is not possible to eliminate nominations, bookings, or technical capacities from the model since they are decided on at different levels of our multilevel model.

Using the latter result, we now introduce additional constraints that bound the technical capacity of a node.

Lemma 3.4 *There exists an optimal solution of the bilevel problem (4) that satisfies (10)–(12) as well as the inequalities*

$$q_u^{TC} \leq |\mathcal{P}_u| \sum_{v \in V_-} q_v^{TC}, \quad u \in V_+ \tag{13a}$$

$$q_u^{TC} \le |\mathcal{P}_u| \sum_{v \in V_+} q_v^{TC}, \quad u \in V_-. \tag{13b}$$

Proof From Lemma 3.3 it follows that an optimal solution of (4) exists that satisfies (10)–(12). Let $t \in T$ be an arbitrary time period and $i \in \mathcal{P}_u$ an arbitrary player at node $u \in V_+ \cup V_-$. From Constraint (5c), we obtain $q_{i,t}^{\text{nom}} \le q_i^{\text{book}}$. Furthermore, from Constraint (5d) it follows

$$q_{i,t}^{\text{nom}} \le \sum_{v \in V_-} \sum_{j \in \mathcal{P}_v} q_{j,t}^{\text{nom}}$$

in case of a gas seller at $u \in V_+$ and

$$q_{i,t}^{\text{nom}} \le \sum_{v \in V_+} \sum_{j \in \mathcal{P}_v} q_{j,t}^{\text{nom}}$$

in case of a gas buyer at $u \in V_-$. Moreover, a time period $l \in T$ with $q_{i,l}^{\text{nom}} = q_i^{\text{book}}$ exists due to Lemma 3.2. From this and Lemma 3.3, we obtain

$$q_{i,t}^{\text{nom}} \le q_{i,l}^{\text{nom}} = q_i^{\text{book}} \le \sum_{v \in V_-} \sum_{j \in \mathcal{P}_v} q_{j,l}^{\text{nom}} \le \sum_{v \in V_-} \sum_{j \in \mathcal{P}_v} q_j^{\text{book}} = \sum_{v \in V_-} q_v^{\text{TC}}$$

in case of $u \in V_+$ and

$$q_{i,t}^{\text{nom}} \le q_{i,l}^{\text{nom}} = q_i^{\text{book}} \le \sum_{v \in V_+} \sum_{j \in \mathcal{P}_v} q_{j,l}^{\text{nom}} \le \sum_{v \in V_+} \sum_{j \in \mathcal{P}_v} q_j^{\text{book}} = \sum_{v \in V_+} q_v^{\text{TC}}$$

in case of $u \in V_-$. Consequently, the claim follows from summing up the previous inequalities w.r.t. $i \in \mathcal{P}_u$ and again using Lemma 3.3. □

We note that the Constraints (13) can be valuable for finding good upper bounds of the technical capacities since gas networks usually contain a small number of entry nodes and very few single players at the nodes. We finally introduce upper bounds for the technical capacity of a node, which depend on the pressure bounds and which can be computed a priori.

Lemma 3.5 *There exists an optimal solution of the bilevel problem (4) satisfying (10)–(13) as well as the constraints*

$$\begin{aligned} q_u^{TC} &\le |\mathcal{P}_u| \left(\sum_{(u,v) \in \delta^{\text{out}}(u)} \sqrt{\frac{(p_u^+)^2 - (p_v^-)^2}{\Lambda_{(u,v)}}} + \sum_{(v,u) \in \delta^{\text{in}}(u)} \sqrt{\frac{(p_u^+)^2 - (p_v^-)^2}{\Lambda_{(v,u)}}} \right) \\ &=: M_u^+, \quad u \in V_+, \end{aligned} \tag{14a}$$

$$\begin{aligned} q_u^{TC} &\le |\mathcal{P}_u| \left(\sum_{(u,v) \in \delta^{\text{out}}(u)} \sqrt{\frac{(p_v^+)^2 - (p_u^-)^2}{\Lambda_{(u,v)}}} + \sum_{(v,u) \in \delta^{\text{in}}(u)} \sqrt{\frac{(p_v^+)^2 - (p_u^-)^2}{\Lambda_{(v,u)}}} \right) \\ &=: M_u^-, \quad u \in V_-. \end{aligned} \tag{14b}$$

Proof From Lemma 3.4, it follows that an optimal solution of (4) exists that satisfies (10)–(13). Let $u \in V_+$. Then, for any feasible point (q^{nom}, q, p) of (1)–(3) and time period $t \in T$, it follows

$$q_{(u,v),t} \le \sqrt{((p_u^+)^2 - (p_v^-)^2)/\Lambda_{(u,v)}}, \quad (u,v) \in \delta^{\text{out}}(u),$$

$$-q_{(v,u),t} \leq \sqrt{((p_u^+)^2 - (p_v^-)^2)/\Lambda_{(v,u)}}, \quad (v,u) \in \delta^{\text{in}}(u).$$

Due to this and (2), it follows

$$\sum_{i \in \mathcal{P}_u} q_{i,t}^{\text{nom}} = \sum_{a \in \delta^{\text{out}}(u)} q_{a,t} - \sum_{a \in \delta^{\text{in}}(u)} q_{a,t} \leq \frac{1}{|\mathcal{P}_u|} M_u^+.$$

Consequently, from this, (11), and (12), it follows

$$q_u^{\text{TC}} = \sum_{i \in \mathcal{P}_u} q_i^{\text{book}} = \sum_{i \in \mathcal{P}_u} \max_{t \in T} \{q_{i,t}^{\text{nom}}\} \leq M_u^+.$$

Analogously, one can show (14b). □

Now, we have derived bounds for the booking price floors, see Lemma 3.1, as well as for the bookings, respectively technical capacities, see Lemma 3.5. These bounds are very important for handling the bilinear terms $\underline{\pi}_u^{\text{book}} q_u^{\text{book}}$ in Constraint (4c). Later on, we handle these bilinear terms with the help of Gurobi [16], which uses McCormick envelopes [25] and spatial branching. For the latter, bounds for $\underline{\pi}_u^{\text{book}}$ and q_u^{book} are necessary.

Moreover, we now can equivalently replace the complementarity constraints (8) by using the standard big-M method. Consequently, we obtain a single-level problem that is larger than the bilevel problem (4) with additional continuous and binary variables and constraints. We note that this single-level problem contains nonsmooth and nonconvex terms in the objective function as well as in Constraint (4c).

We emphasize that the obtained single-level reformulation is still computationally intractable since it contains the infinitely many nonlinear adjustable robust constraints (4d) that model technical capacities. We now tackle these constraints in the next section and show that we can model their feasible region by finitely many convex constraints including integer variables.

4 Handling technical capacities in trees

In this section, we provide a finite-dimensional model for the infinitely many nonlinear adjustable robust constraints (4d) for the case of tree-shaped networks. Since these adjustable robust constraints are very challenging, especially for the considered nonlinear gas transport model (1)–(3), we assume that the graph G is a tree throughout this section.

We first introduce some necessary notation, which is mainly taken from [31]. Using directed graphs to represent gas networks is a modeling choice that allows to interpret the direction of flows. However, the flow in a gas network is not influenced by the direction of the arcs. Thus, for $u, v \in V$, we introduce so-called *flow-paths* $P := P(u,v) = (V(u,v), A(u,v))$ in which $V(u,v) \subseteq V$ contains the nodes of the path from u to v in the undirected version of the graph G and $A(u,v) \subseteq A$ contains the corresponding arcs of this path. Consequently, a flow-path can be interpreted as an undirected path that additionally contains for each arc its direction in the original network $G = (V, A)$. The latter allows us to determine the flow direction for an arc. For another pair of nodes $u', v' \in V$, we say that $P(u',v')$ is a *flow-subpath* of $P(u,v)$ if $P(u',v') \subseteq P(u,v)$, i.e., $V(u',v') \subseteq V(u,v)$ and $A(u',v') \subseteq A(u,v)$, holds and if $P(u',v')$ is itself a flow-path.

We now focus on tree-shaped networks and thus, the flow-path between two nodes is unique. For modeling reasons, we partition the arcs of a given flow-path $P(u,v)$ into $A^{\rightarrow}(u,v)$ and $A^{\leftarrow}(u,v)$. The set $A^{\rightarrow}(u,v)$ contains all arcs of $P(u,v)$ that are directed from u to v, i.e., an arc $(u', v') \in A^{\rightarrow}(u, v)$ satisfies $P(v', v) \subset P(u', v)$. The remaining arcs of the flow-path $P(u, v)$ are contained in $A^{\leftarrow}(u, v)$. We note that for a fixed node pair these arc sets are unique due to the tree structure of the graph. We can also compute them for every flow-path a priori by depth-first search.

Finally, for a tree-shaped network and arc $a = (u, v) \in A$, we now introduce two sub-graphs that are later used to determine the maximal flow on an arc. If we delete arc a in G, then the tree decomposes into two sub-trees. We define the sub-tree including node u as $G_u = (V_u^{(u,v)}, A_u^{(u,v)})$ and the other sub-tree, which contains v, as $G_v = (V_v^{(u,v)}, A_v^{(u,v)})$. Due to this construction, $V_v^{(u,v)} = V \setminus V_u^{(u,v)}$ holds.

The outline to derive a finite-dimensional reformulation of the computational intractable nonlinear adjustable constraint (4d) is as follows. We first state a known characterization for technical capacities that enables us to verify the feasibility of technical capacities by solving, for each pair of nodes, a nonlinear optimization problem to global optimality. We then exploit monotonicity properties of these nonlinear problems together with certain flow properties in tree-shaped networks to model the corresponding optimal value functions by finitely many convex constraints including newly introduced binary variables.

From Theorem 10 in [21], it follows that we can verify the feasibility of given technical capacities by solving a nonlinear optimization problem for each pair of nodes $(w_1, w_2) \in V^2$. One of these nonlinear problems computes the maximal pressure difference between the considered nodes w_1 and w_2 within the given technical capacities and is composed of

$$\triangle_{(w_1,w_2)}(q^{\mathrm{TC}}) := \max_{q^{\mathrm{nom}},q,p} \quad p_{w_1}^2 - p_{w_2}^2 \tag{15a}$$

$$\text{s.t.} \quad \sum_{a \in \delta^{\mathrm{out}}(u)} q_a - \sum_{a \in \delta^{\mathrm{in}}(u)} q_a = \sum_{i \in \mathcal{P}_u} q_i^{\mathrm{nom}}, \quad u \in V_+, \tag{15b}$$

$$\sum_{a \in \delta^{\mathrm{out}}(u)} q_a - \sum_{a \in \delta^{\mathrm{in}}(u)} q_a = -\sum_{i \in \mathcal{P}_u} q_i^{\mathrm{nom}}, \quad u \in V_-, \tag{15c}$$

$$\sum_{a \in \delta^{\mathrm{out}}(u)} q_a - \sum_{a \in \delta^{\mathrm{in}}(u)} q_a = 0, \quad u \in V_0, \tag{15d}$$

$$p_u^2 - p_v^2 = \Lambda_a q_a \, |q_a|, \quad a = (u, v) \in A, \tag{15e}$$

$$q^{\mathrm{nom}} \in \mathcal{N}(q^{\mathrm{TC}}). \tag{15f}$$

We note that Constraints (15b)–(15e) are the same as Constraints (2) and (3) except that they do not depend on the specific time step anymore since the technical capacities are determined once for all time steps.

It is shown in Theorem 10 of [21] that feasible technical capacities can be characterized by constraints on the maximum pressure difference between all pairs of nodes, i.e., by constraints on the objective value of (15).

Lemma 4.1 (Theorem 10 in [21]) *Let $G = (V, A)$ be a graph and $q^{TC} \in \mathbb{R}_{\geq 0}^{V_+ \cup V_-}$. Then, q^{TC} satisfies Constraint (4d) if and only if for each node pair $(w_1, w_2) \in V^2$ the corresponding optimal value of (15) satisfies*

$$\triangle_{(w_1,w_2)}(q^{TC}) \leq (p_{w_1}^+)^2 - (p_{w_2}^-)^2. \tag{16}$$

We note that this characterization allows us to replace the nonlinear adjustable robust constraint (4d) by (16). For tree-shaped networks, it is further proven in [21] that the optimal value function $\triangle_{w_1,w_2}(q^{\mathrm{TC}})$ can be modeled by exploiting the following flow bounds that depend on given technical capacities.

Lemma 4.2 (Lemma 3.2 in [31]) *Let $G = (V, A)$ be a tree, $q^{TC} \in \mathbb{R}^{V_+ \cup V_-}$ technical capacities, $q^{\text{nom}} \in \mathcal{N}(q^{TC})$ a nomination, and q its unique flow given by (2). Then, for every arc $a = (u, v) \in A$, the flow q_a is bounded by*

$$\begin{aligned} \xi_a^-(q^{TC}) &:= -\min\left\{ \sum_{w \in V_+ \cap V_v^{(u,v)}} q_w^{TC}, \sum_{w \in V_- \cap V_u^{(u,v)}} q_w^{TC} \right\} \le q_a, \\ q_a &\le \min\left\{ \sum_{w \in V_+ \cap V_u^{(u,v)}} q_w^{TC}, \sum_{w \in V_- \cap V_v^{(u,v)}} q_w^{TC} \right\} =: \xi_a^+(q^{TC}). \end{aligned} \tag{17}$$

Moreover, it is shown in [21], respectively in Lemmas 3.4 and 3.5 of [31] by using an alternative proof technique, that these flow bounds are tight for all arcs of a given flow-path. Consequently, the optimal value function $\triangle_{w_1,w_2}(q^{\text{TC}})$ can be explicitly expressed as follows, which has been shown in Corollary 19 in [21] in a slightly modified setting.

Lemma 4.3 (Corollary 19 in [21]) *Let $G = (V, A)$ be a tree, $q^{TC} \in \mathbb{R}^{V_+ \cup V_-}$ technical capacities, and $w_1, w_2 \in V$. Then,*

$$\triangle_{w_1,w_2}(q^{TC}) = \sum_{a \in A^{\rightarrow}(w_1,w_2)} \Lambda_a \xi_a^+(q^{TC})^2 + \sum_{a \in A^{\leftarrow}(w_1,w_2)} \Lambda_a \xi_a^-(q^{TC})^2 \tag{18}$$

holds, where $\xi_a^+(q^{TC})$ and $\xi_a^-(q^{TC})$ are the upper and lower arc flow bounds given by (17).

This explicit representation of the optimal value function $\triangle_{w_1,w_2}(q^{\text{TC}})$ allows us to simplify the characterization for technical capacities of Lemma 4.1.

Corollary 4.4 *Let $G = (V, A)$ be a graph and $q^{TC} \in \mathbb{R}_{\ge 0}^{V_+ \cup V_-}$. Then, q^{TC} satisfies Constraint (4d) if and only if for each node pair $(w_1, w_2) \in V^2$ the constraint*

$$\sum_{a \in A^{\rightarrow}(w_1,w_2)} \Lambda_a \xi_a^+(q^{TC})^2 + \sum_{a \in A^{\leftarrow}(w_1,w_2)} \Lambda_a \xi_a^-(q^{TC})^2 \le (p_{w_1}^+)^2 - (p_{w_2}^-)^2 \tag{19}$$

is fulfilled, where $\xi_a^+(q^{TC})$ and $\xi_a^-(q^{TC})$ are the upper and lower arc flow bounds given by (17).

We now can replace the nonlinear adjustable robust constraint (4d) that models feasible technical capacities by our simplified characterization (19). To do so, we present a model for this simplified characterization (19) that consists of finitely-many convex constraints including newly introduced integer variables. For stating the model, we first need to bound the technical capacities. From Lemma 3.5, it follows that an optimal solution of the bilevel problem (4) exists such that the technical capacity of a node is bounded above by M_u^+ for all $u \in V_+$ and by M_u^- for all $u \in V_-$. Consequently, we can bound the aggregated technical capacities of all entries, respectively exits, by

$$M^+ := \sum_{u \in V_+} M_u^+ \ge \sum_{u \in V_+} q_u^{\text{TC}}, \tag{20a}$$

$$M^- := \sum_{u \in V_-} M_u^- \ge \sum_{u \in V_-} q_u^{\text{TC}}. \tag{20b}$$

We note that the bilinear terms of the following model can be reformulated by using big-Ms, which we describe later. Our convex mixed-integer model of (19) is given as follows:

$$\bar{h}^+_{(u,v)} = \sum_{w \in V_+ \cap V_u^{(u,v)}} q_w^{\mathrm{TC}}, \qquad (u,v) \in A, \tag{21a}$$

$$\bar{h}^-_{(u,v)} = \sum_{w \in V_- \cap V_v^{(u,v)}} q_w^{\mathrm{TC}}, \qquad (u,v) \in A, \tag{21b}$$

$$\bar{h}^+_{(u,v)} - \bar{h}^-_{(u,v)} \leq M^+ \bar{x}_{(u,v)}, \qquad (u,v) \in A, \tag{21c}$$

$$\bar{q}_{(u,v)} = \bar{h}^+_{(u,v)}(1 - \bar{x}_{(u,v)}) + \bar{h}^-_{(u,v)} \bar{x}_{(u,v)}, \qquad (u,v) \in A, \tag{21d}$$

$$\underline{h}^+_{(u,v)} = \sum_{w \in V_+ \cap V_v^{(u,v)}} q_w^{\mathrm{TC}}, \qquad (u,v) \in A, \tag{21e}$$

$$\underline{h}^-_{(u,v)} = \sum_{w \in V_- \cap V_u^{(u,v)}} q_w^{\mathrm{TC}}, \qquad (u,v) \in A, \tag{21f}$$

$$\underline{h}^+_{(u,v)} - \underline{h}^-_{(u,v)} \leq M^+ \underline{x}_{(u,v)}, \qquad (u,v) \in A, \tag{21g}$$

$$\underline{q}_{(u,v)} = \underline{h}^+_{(u,v)}(1 - \underline{x}_{(u,v)}) + \underline{h}^-_{(u,v)} \underline{x}_{(u,v)}, \qquad (u,v) \in A, \tag{21h}$$

$$\bar{q}_a^2 \leq \bar{f}_a, \qquad a \in A, \tag{21i}$$

$$\underline{q}_a^2 \leq \underline{f}_a, \qquad a \in A, \tag{21j}$$

$$\sum_{a \in A^{\rightarrow}(u,v)} \Lambda_a \bar{f}_a + \sum_{a \in A^{\leftarrow}(u,v)} \Lambda_a \underline{f}_a \leq (p_u^+)^2 - (p_v^-)^2, \qquad (u,v) \in V^2, \tag{21k}$$

$$\underline{x}_a, \bar{x}_a \in \{0,1\}, \; q_v^{\mathrm{TC}} \geq 0, \qquad a \in A, \; v \in V. \tag{21l}$$

Constraints (21a)–(21d) and (21e)–(21h) ensure that $\bar{q}$ is at least as large as the upper flow bound $\xi_a^+(q^{\mathrm{TC}})$ and $\underline{q}$ is at least the absolute value of the lower flow bound $\xi_a^-(q^{\mathrm{TC}})$; see Lemma 4.2. The negative sign of the lower flow bound is directly modeled in Constraints (21k). Constraints (21i) and (21j) result from a modeling choice. They allow to model the flow linearly in Constraints (21k), which reduces the number of convex constraints.

We now show the correctness of (21). To this end, we first prove that any feasible point of the original bilevel problem (4) satisfying Lemma 3.5 can be extended to a feasible point of (21). Afterward, we prove that every feasible point of (21) is also feasible for the adjustable robust constraint (4d) of the bilevel problem (4). We abbreviate a feasible point of (21) by z, i.e.,

$$z = \left(\bar{f}, \underline{f}, \bar{q}, \underline{q}, \underline{h}^-, \bar{h}^-, \underline{h}^+, \bar{h}^+, \underline{x}, \bar{x}, q^{\mathrm{TC}}\right).$$

Lemma 4.5 *Let $G = (V, A)$ be a tree and $q^{TC} \in \mathbb{R}_{\geq 0}^{V_+ \cup V_-}$ be part of an optimal solution of (4) satisfying Lemma 3.5. Then, q^{TC} can be extended to a feasible point z of (21).*

Proof Constraints (21a), (21b), (21e), and (21f) are uniquely determined by q^{TC}. Further, they are feasible because the corresponding variables are not bounded. Due to the construction of M^+ by (20a) and (20b), we can set for $a \in A$ the variable $\bar{x}_a$, respectively $\underline{x}_a$, to 1 if the left-hand side of (21c), respectively (21g), is positive and otherwise to 0. Due to this assignment, $\bar{q}_a$ is uniquely determined and equals the upper flow bound $\xi_a^+(q^{\mathrm{TC}})$; see (17). Further, $\underline{q}_a$ is unique and equals the absolute value of the lower flow bound $\xi_a^-(q^{\mathrm{TC}})$; see (17). We now set $\bar{f}_a = \bar{q}_a^2$, respectively $\underline{f}_a = \underline{q}_a^2$, for $a \in A$ and thus, Constraints (21i) and (21j) are satisfied.

Finally, we have to check the feasibility of Constraints (21k). For doing so, we consider an arbitrary node pair $(u, v) \in V^2$. From the previous construction it follows that (21k) simplifies to

$$\sum_{a \in A^{\rightarrow}(u,v)} \Lambda_a \bar{f}_a + \sum_{a \in A^{\leftarrow}(u,v)} \Lambda_a \underline{f}_a = \sum_{a \in A^{\rightarrow}(u,v)} \Lambda_a \xi_a^+ (q^{\mathrm{TC}})^2 + \sum_{a \in A^{\leftarrow}(u,v)} \Lambda_a \xi_a^- (q^{\mathrm{TC}})^2$$
$$\leq (p_u^+)^2 - (p_v^-)^2.$$

The feasibility of the last inequality follows from Corollary 4.4 and the feasibility of the considered technical capacities q^{TC} for (4d). Consequently, the constructed point is feasible for (21). □

We now prove that a feasible point of (21) is also feasible to the adjustable robust constraint (4d).

Lemma 4.6 *Let $G = (V, A)$ be a tree and let z be a feasible point of (21). Then, q^{TC} satisfies (4d).*

Proof We contrarily assume that q^{TC} does not satisfy Constraint (4d). Thus, from Corollary 4.4 it follows that there is a node pair $(w_1, w_2) \in V^2$ violating (19), i.e.,

$$\sum_{a \in A^{\rightarrow}(w_1,w_2)} \Lambda_a \xi_a^+ (q^{\mathrm{TC}})^2 + \sum_{a \in A^{\leftarrow}(w_1,w_2)} \Lambda_a \xi_a^- (q^{\mathrm{TC}})^2 > (p_{w_1}^+)^2 - (p_{w_2}^-)^2. \tag{22}$$

Due to Constraints (21a)–(21d), it follows

$$\xi_a^+ (q^{\mathrm{TC}})^2 \leq \bar{q}_a^2 \leq \bar{f}_a, \; a \in A^{\rightarrow}(u, v), \quad \xi_a^- (q^{\mathrm{TC}})^2 \leq \underline{q}_a^2 \leq \bar{f}_a, \; a \in A^{\leftarrow}(u, v).$$

Consequently, from this and the feasibility of (21k) for z, it follows

$$\sum_{a \in A^{\rightarrow}(w_1,w_2)} \Lambda_a \xi_a^+ (q^{\mathrm{TC}})^2 + \sum_{a \in A^{\leftarrow}(w_1,w_2)} \Lambda_a \xi_a^- (q^{\mathrm{TC}})^2$$
$$\leq \sum_{a \in A^{\rightarrow}(w_1,w_2)} \Lambda_a \bar{f} + \sum_{a \in A^{\leftarrow}(w_1,w_2)} \Lambda_a \underline{f} \leq (p_{w_1}^+)^2 - (p_{w_2}^-)^2,$$

which is a contradiction to (22). □

Combining the previous results proves that we can model the infinitely many adjustable robust constraints (4d) by the finitely many Constraints (21).

Theorem 4.7 *Let $G = (V, A)$ be a tree. Then, every optimal solution of the bilevel problem (4), where we replaced (4d) by (21), is an optimal solution of the bilevel problem (4). Moreover, every optimal solution of (4) that additional satisfies the conditions of Lemma 3.5 can be extended to an optimal solution of (4), where we replaced (4d) by (21).*

Proof The claim follows from Lemmas 3.5, 4.5, and 4.6 . □

Remark 4.8 We note that we can easily include lower q_a^- and upper q_a^+ arc flow bounds for all arcs $a \in A$ by

$$q_a^- \leq -\underline{q}_a \leq q_a^+, \quad q_a^- \leq \bar{q}_a \leq q_a^+.$$

Since in Model (21) the variable $\underline{q}_a$ equals the absolute value of the lower arc flow bound $\xi_a^-(q^{\mathrm{TC}})$ and since $\bar{q}_a$ equals the upper arc flow bound $\xi_a^+(q^{\mathrm{TC}})$ given by Lemma 4.2, this ensures that the flow stays in the a priori given flow bounds. We abstract from flow bounds in our model, since the consideration of pressure levels allows to bound the flow by Constraints (21k).

Model (21) contains bilinear terms in Constraints (21d) and (21h). Since these bilinear terms are products of a binary variable and a nonnegative and bounded variable, we can reformulate them using big-Ms. We note that the upper bounds for $\underline{h}^+_{(u,v)}$ and $\bar{h}^+_{(u,v)}$ are given by (20a) and for $\bar{h}^-_{(u,v)}$ and $\underline{h}^-_{(u,v)}$ by (20b). The bilinear constraints (21d) can thus be reformulated as

$$\bar{q}_{(u,v)} = \bar{y}^+_{(u,v)} + \bar{y}^-_{(u,v)}, \tag{23a}$$

$$\bar{y}^+_{(u,v)} \geq 0, \quad \bar{y}^+_{(u,v)} \leq M^+(1 - \bar{x}_{(u,v)}), \quad \bar{y}^+_{(u,v)} \geq \bar{h}^+_{(u,v)} - M^+\bar{x}_{(u,v)}, \tag{23b}$$

$$\bar{y}^-_{(u,v)} \geq 0, \quad \bar{y}^-_{(u,v)} \leq M^-\bar{x}_{(u,v)}, \quad \bar{y}^-_{(u,v)} \geq \bar{h}^-_{(u,v)} - M^-(1 - \bar{x}_{(u,v)}). \tag{23c}$$

In analogy, we can reformulate the bilinear constraints (21h) by

$$\underline{q}_{(u,v)} = \underline{y}^+_{(u,v)} + \underline{y}^-_{(u,v)}, \tag{24a}$$

$$\underline{y}^+_{(u,v)} \geq 0, \quad \underline{y}^+_{(u,v)} \leq M^+(1 - \underline{x}_{(u,v)}), \quad \underline{y}^+_{(u,v)} \geq \underline{h}^+_{(u,v)} - M^+\underline{x}_{(u,v)}, \tag{24b}$$

$$\underline{y}^-_{(u,v)} \geq 0, \quad \underline{y}^-_{(u,v)} \leq M^-\underline{x}_{(u,v)}, \quad \underline{y}^-_{(u,v)} \geq \underline{h}^-_{(u,v)} - M^-(1 - \underline{x}_{(u,v)}). \tag{24c}$$

For ease of notation in the following lemma, (21*) denotes (21) where we replaced Constraints (21d) and (21h) by (23) and (24).

Lemma 4.9 *A vector $q^{TC} \in \mathbb{R}^{V_+ \cup V_-}_{\geq 0}$ is feasible for (21) if and only if it is feasible for (21*).*

Proof We can extend every feasible solution of (21) to satisfy (23) and (24). To do so, we choose $\bar{y}^+$, $\bar{y}^-$, $\underline{y}^+$, and $\underline{y}^+$ as small as possible. Consequently, (23a) and (24a) equal Constraints (21d) and (21h). Thus, the extended solution satisfies (21*).

From the construction of (23) and (24) it follows that the flows $\bar{q}$ and $\underline{q}$ obtained in (23a) and (24a) are at least as large as the flows obtained in (21d) and (21h). From this and the fact that $\Lambda_a q_a |q_a|$ is increasing for all $a \in A$, it follows that every feasible point of (21*), is also feasible for (21). □

After reformulating the bilinear terms in (21) by the discussed linearizations, we can model the adjustable robust Constraint (4d) by the finitely many constraints

$$(21a)\text{–}(21c),\ (21e)\text{–}(21g),\ (21i)\text{–}(21l),\ (23),\ (24). \tag{25}$$

For the considered nonlinear flow model, which is based on the Weymouth pressure loss equation, the presented model of the technical capacities is a convex mixed-integer model. This is surprising since the Weymouth pressure drop model is itself nonconvex. The convex mixed-integer reformulation is obtained by using additional binary variables to model the maximum flow in a pipe and by exploiting that, for the considered gas transport model, the pressure drop $\Lambda_a q_a |q_a|$ is quadratic for every pipe $a \in A$ if the direction of the arc flow q_a is known. The model further consists only of polynomially many (in the number of nodes of the network) constraints and variables. Finally, we note that this model can also be generalized to potential-based flow models as explained in Remark 2.1. To do so, we only have to replace (21k) by

$$\sum_{a \in A^{\rightarrow}(u,v)} \phi_a(\bar{q}_a) + \sum_{a \in A^{\leftarrow}(u,v)} \phi_a(\underline{q}_a) \leq \pi^+_u - \pi^-_v, \quad (u, v) \in V^2,$$

where ϕ is the potential loss function as introduced in Remark 2.1. We further can neglect Constraints (21i) and (21j), which result from a modeling choice to reduce the number of convex constraints. For general potential-based flows, the obtained model is not necessarily convex anymore since general potential loss functions may not depend quadratically on the arc flow, e.g., in case of water networks.

5 Additional combinatorial constraints

In this section, we present valid combinatorial constraints for (21), respectively (25), that speed up the solution process, which we will analyze later in Sect. 6. We prove the results w.r.t. Model (21), but they can be shown in analogy for Model (25). We note that these additional constraints do not influence the set of feasible technical capacities modeled by (21).

We first prove that for every feasible point z of (21), a feasible point with the same technical capacities q^{TC} always exists such that the right-hand sides of Constraints (21c) and (21g) are minimal, i.e., a binary variable is zero if the corresponding left-hand side is non-positive. Here, $\lceil x \rceil$ denotes rounding up the value x.

Lemma 5.1 *Let $G = (V, A)$ be a tree and let z be a feasible point of (21) with technical capacities q^{TC}. Then, a feasible point $\tilde{z}$ with the same technical capacities q^{TC} exists such that for arc $(u, v) \in A$ the corresponding binaries are given by*

$$\bar{\tilde{x}}_{(u,v)} = \max\left\{0, \left\lceil \frac{1}{M^+}(\bar{h}^+_{(u,v)} - \bar{h}^-_{(u,v)}) \right\rceil \right\}, \tag{26a}$$

$$\underline{\tilde{x}}_{(u,v)} = \max\left\{0, \left\lceil \frac{1}{M^+}(\underline{h}^+_{(u,v)} - \underline{h}^-_{(u,v)}) \right\rceil \right\}. \tag{26b}$$

Proof Let be $z = (\bar{f}, \underline{f}, \bar{q}, \underline{q}, \underline{h}^-, \bar{h}^-, \underline{h}^+, \bar{h}^+, \underline{x}, \bar{x}, q^{\mathrm{TC}})$ a feasible point of (21). We assume that an arc $(u, v) \in A$ exists such that, w.l.o.g.,

$$1 = \bar{x}_{(u,v)} > 0 = \max\left\{0, \left\lceil \frac{1}{M^+}(\bar{h}^+_{(u,v)} - \bar{h}^-_{(u,v)}) \right\rceil \right\}$$

holds. We now set $\bar{x}_{(u,v)} = 0$. Consequently, $\bar{q}_{(u,v)}$ possibly decreases according to Constraint (21d). The remaining point stays feasible since Constraints (21a), (21b), (21e)–(21h), (21j), and (21l) are not affected by this modification. Furthermore, Constraint (21i) is still fulfilled since we only possibly decreased $\bar{q}_{(u,v)}$ and thus, (21k) is satisfied. We also note that Constraint (21c) is satisfied due to the choice of $M^+ \geq 0$.

Repeating the previous procedure for $\bar{x}$ and $\underline{x}$ shows the claim. □

With the help of the latter result, we now present additional combinatorial constraints regarding the binary variables that explicitly use the network structure. The intuition behind these constraints can be sketched as follows: From Lemma 5.1 it follows that an optimal solution for model (21) exists such that for an arc $a = (u, v) \in A$, the variable $\bar{q}_a$ represents the maximal arc flow of a, i.e.,

$$\bar{q}_{(u,v)} = \min\left\{ \sum_{w \in V_+ \cap V_u^{(u,v)}} q_w^{\mathrm{TC}}, \sum_{w \in V_- \cap V_v^{(u,v)}} q_w^{\mathrm{TC}} \right\} = \min\left\{\bar{h}^+_{(u,v)}, \bar{h}^-_{(u,v)}\right\}.$$

This means that $\bar{q}_a$ equals the minimum flow that can be sent via (u, v) by entries in $V_u^{(u,v)}$, which is the sub-tree that includes node u and is obtained by removing arc (u, v), and of the flow that can be received by exits in $V_v^{(u,v)}$. If the entries in $V_u^{(u,v)}$ can supply more flow than the exits in $V_v^{(u,v)}$ can receive, i.e.,

$$\bar{q}_{(u,v)} = \min\left\{\sum_{w\in V_+\cap V_u^{(u,v)}} q_w^{\mathrm{TC}}, \sum_{w\in V_-\cap V_v^{(u,v)}} q_w^{\mathrm{TC}}\right\} = \sum_{w\in V_-\cap V_v^{(u,v)}} q_w^{\mathrm{TC}} = \bar{h}^-_{(u,v)},$$

then $\bar{x}_{(u,v)} = 1$ holds. Considering now for an outgoing arc (v,l) the variable $\bar{q}_{(v,l)}$ only possibly increases the number of entries that can supply flow via (v,l), i.e., $V_u^{(u,v)} \subset V_v^{(v,l)}$, and possibly reduces the number of exits that can receive flow via arc (v,l), i.e., $V_l^{(v,l)} \subset V_v^{(u,v)}$. Consequently, the value of $\bar{q}_{(v,l)}$ is again determined by the exits, i.e., $\bar{q}_{(v,l)} = \bar{h}^-_{(v,l)}$, and, thus, $\bar{x}_{(v,l)} = 1$ holds. This shows a correspondence between the binary variables using the given network structure and is the key for the following combinatorial constraints. In analogy to the above, we can derive further constraints for the binaries $\underline{x}$ corresponding to the lower flow variables $\underline{q}$.

Lemma 5.2 *Let $G = (V, A)$ be a tree and z a feasible point of (21) that satisfies (26). Then, the inequalities*

$$\bar{x}_{(u,v)} \le \bar{x}_{(v,l)}, \quad (v,l) \in \delta^{\mathrm{out}}(v), \tag{27a}$$
$$\underline{x}_{(v,l)} \le \underline{x}_{(u,v)}, \quad (v,l) \in \delta^{\mathrm{out}}(v), \tag{27b}$$
$$\bar{x}_{(u,v)} \le \underline{x}_{(l,v)}, \quad (l,v) \in \delta^{\mathrm{in}}(v), \tag{27c}$$

are satisfied for $a = (u, v)$.

Proof Applying Lemma 5.1, a feasible point $(\bar{f}, \underline{f}, \bar{q}, \underline{q}, \underline{h}^-, \bar{h}^-, \underline{h}^+, \bar{h}^+, \underline{x}, \bar{x}, q^{\mathrm{TC}})$ for (21) exists that satisfies (26).

We first consider Inequality (27a). If $\bar{x}_{(u,v)} = 0$ holds, then (27a) is redundant since $\bar{x}_{(v,l)} \in \{0, 1\}$. We now assume that $\bar{x}_{(u,v)} = 1$ holds. Consequently,

$$1 = \bar{x}_{(u,v)} = \left\lceil \frac{1}{M^+}(\bar{h}^+_{(u,v)} - \bar{h}^-_{(u,v)}) \right\rceil$$

holds and thus,

$$\bar{h}^+_{(u,v)} > \bar{h}^-_{(u,v)} \ge 0$$

is satisfied. From $(v,l) \in \delta^{\mathrm{out}}(v)$ it follows

$$V_u^{(u,v)} \subset V_v^{(v,l)}, \quad V_l^{(v,l)} \subset V_v^{(u,v)}, \tag{28}$$

where $V_u^{(u,v)}$, respectively $V_v^{(v,l)}$, contains the nodes of the connected component that includes u, respectively v, and is created by removing arc (u,v), respectively (v,l). From this as well as Constraints (21a) and (21b), it follows

$$\bar{h}^+_{(v,l)} \ge \bar{h}^+_{(u,v)} > \bar{h}^-_{(u,v)} \ge \bar{h}^-_{(v,l)} \ge 0,$$

and consequently, $\bar{x}_{(v,l)} = 1$ is satisfied due to (21c).

We now consider (27b). If $\underline{x}_{(v,l)} = 0$ holds, then (27b) is redundant since $\underline{x}_{(u,v)} \in \{0, 1\}$. Thus, we now assume that $\underline{x}_{(v,l)} = 1$ holds. Due to (26),

$$1 = \underline{x}_{(v,l)} = \left\lceil \frac{1}{M^+}(\underline{h}^+_{(v,l)} - \underline{h}^-_{(v,l)}) \right\rceil$$

holds and, thus,

$$\underline{h}^{+}_{(v,l)} > \underline{h}^{-}_{(v,l)} \geq 0$$

is satisfied. From $(v, l) \in \delta^{\text{out}}(v)$ it again follows (28). This, as well as Constraints (21e) and (21f), lead to

$$\underline{h}^{+}_{(u,v)} \geq \underline{h}^{+}_{(v,l)} > \underline{h}^{-}_{(v,l)} \geq \underline{h}^{-}_{(u,v)} \geq 0,$$

and consequently, $\underline{x}_{(u,v)} = 1$ is satisfied due to (21g).

We finally consider (27c). If $\bar{x}_{(u,v)} = 0$ holds, then (27c) is redundant since $\underline{x}_{(l,v)} \in \{0, 1\}$. Thus, we now assume that $\bar{x}_{(u,v)} = 1$ holds. Due to (26),

$$1 = \bar{x}_{(u,v)} = \left\lceil \frac{1}{M}(\bar{h}^{+}_{(u,v)} - \bar{h}^{-}_{(u,v)}) \right\rceil$$

holds and, thus,

$$\bar{h}^{+}_{(u,v)} > \bar{h}^{-}_{(u,v)} \geq 0$$

is satisfied.

From $(l, v) \in \delta^{\text{in}}(v)$, it follows

$$V_u^{(u,v)} \subset V_v^{(l,v)}, \quad V_l^{(l,v)} \subset V_v^{(u,v)}$$

and thus, from (21a), (21b), (21e), and (21f) it follows

$$\underline{h}^{+}_{(l,v)} \geq \bar{h}^{+}_{(u,v)} > \bar{h}^{-}_{(u,v)} \geq \underline{h}^{-}_{(l,v)} \geq 0.$$

From this and Constraint (21g) it follows $\underline{x}_{(l,v)} = 1$. □

Consequently, the adjustable robust constraint (4d) can be modeled by (21), respectively (25), and the additional Constraints (27a)–(27c). In the following computational study, we demonstrate the impact of the presented combinatorial constraints w.r.t. running times.

6 Computational results

We now apply our results to solve the considered multilevel model of the European entry-exit gas market system with a nonlinear flow model in tree-shaped networks. To this end, we solve the model for a passive version of the Greek gas network, i.e., the network corresponds to the Greek gas network excluding its single compressor station and its single control valve. This is the first time that the considered entry-exit gas market model can be solved for a real-world sized network. For our computations, we consider the single-level reformulation (9) with linearized complementarity constraints, the additional constraints (12) and (13), the handling of the technical capacities (25), and the additional combinatorial constraints (27). For the latter, we also analyze their explicit effect on the running times. We further note that we can a priori exclude Constraints (1) and (3) since the flow is uniquely determined by (2) in tree-shaped networks.

6.1 Physical and economic data

For our computational analysis, we consider the GasLib 134 (version 2) network; see [33]. The GasLib 134 represents the Greek gas network, with more than 7000 km of pipes. It further is the largest publicly available tree-shaped gas network and, thus, we focus on this network in our computational study. Since the integration of active elements is currently out of scope,

Table 1 Economic data for exit demands functions $P_{i,t}(q_{i,t}^{\mathrm{nom}}) = b_i q_{i,t}^{\mathrm{nom}} + a_{i,t}$ with $a_{i,t} = \max_{j \in \mathcal{P}_u, u \in V_+} \{c_j^{\mathrm{var}}\} + h_{i,t}$, where the integer $h_{i,t}$ (in €/(1000 Nm^3/h)) is uniformly sampled in the given intervals and b_i is given in €/(1000 Nm^3/h)^2

$h_{i,0}$	$h_{i,1}$	$h_{i,2}$	$h_{i,3}$	b_i
[5, 20]	[31, 50]	[51, 60]	[31, 40]	−2

we bypass the single compressor station and single control valve of the GasLib 134 network. Moreover, we slightly adapt the lower pressure bounds of the GasLib 134 network by setting all lower pressure bounds of at least 37.5 bar to 32.5 bar. This ensures that the intersection of the lower and the upper pressure bound intervals is non-empty, i.e., $\bigcap_{u \in V_+ \cup V_-} [p_u^-, p_u^+] \neq \emptyset$. The latter is a necessary condition for the existence of a feasible nomination in a passive network. In total, the network consists of 134 nodes, which contain 3 entries, 45 exits, and 86 inner nodes, and 133 pipes, which contain 47 short pipes[2] and 86 pipes. Each pipe $a \in A$ is characterized by its length L_a, diameter D_a, and roughness k_a. Further, we assume that all pipes are horizontal. For each pipe $a \in A$, we compute the pressure loss coefficient Λ_a of the considered Weymouth model (1)–(3) according to (2.25) in [10], i.e.,

$$\Lambda_a = \left(\frac{4}{\pi}\right)^2 \lambda_a \frac{R_{\mathrm{s}} T_{\mathrm{m}} L_a z_{\mathrm{m},a}}{D_a^5}.$$

Here, R_{s} is the specific gas constant, T_{m} a constant mean temperature, λ_a is the friction factor of pipe $a \in A$ computed using the formula of Nikarudse, and $z_{\mathrm{m},a}$ is the mean compressibility factor of a pipe $a \in A$ computed by the formula of Papay and an a priori estimation of the mean pressure; see Chapters [10,30] for the explicit formulas and additional explanations.

We now turn to the modeling of the economic data. The considered time horizon consists of four time periods $t \in T$ that model the seasons summer ($t = 0$), autumn ($t = 1$), winter ($t = 2$), and spring ($t = 3$). In line with [2], we assume a single player per node. We model the variable production costs c_i^{var} of the three existing entries as follows. For entry node_80, we set $c_{\mathrm{node\_80}}^{\mathrm{var}} = 112$€/(1000 Nm^3/h) and then increase this value by 5% for production costs of the remaining entries. In a simplified way, this roughly represents the current situation regarding production costs in the Greek gas network. For the linear demand functions of the exit nodes, we assume

$$P_{i,t}(q_{i,t}^{\mathrm{nom}}) = b_i q_{i,t}^{\mathrm{nom}} + a_{i,t} \quad \text{with} \quad a_{i,t} = \max_{j \in \mathcal{P}_u, u \in V_+} \left\{c_j^{\mathrm{var}}\right\} + h_{i,t},$$

where the integer $h_{i,t}$ is uniformly sampled in certain intervals; see Table 1. This construction explicitly ensures that Assumption 2 is satisfied. We note that $a_{i,t}$ is lowest in the summer ($t = 0$) and highest in the winter ($t = 2$). After fixing the previous values, we consider exogenous network costs $C \in \{0, 5000, 10\,000, \ldots, 30\,000\}$ € and the transport costs $c_t^{\mathrm{trans}} \in \{0.1, 0.2, \ldots, 1.0\}$ €/bar^2. Additionally, for the instances with $C = 15,000$€, we vary the intercepts $a_{i,t}$ by adding a "shift" in $\{-10, -5, 0, 5, 10\}$ €/(1000 Nm^3)/h. In total, we obtain 110 instances.

We note that all these values have to be seen w.r.t. the considered time horizon of 1 h per time period. Moreover, extrapolating the results for the time horizon of a whole year shows

[2] Although the presented theory is stated for the case of pipes with positive pressure loss coefficient $\Lambda_a > 0$, it is no harm to consider short pipes with $\Lambda_a = 0$ since gas pressure levels are not influenced by including short pipes.

that the total gas consumption of the base case, i.e., $C = 15\,000€$ and $c^{\text{var}} = 0.5\,€/\text{bar}^2$ deviates by less than 1.4% from the total gas consumption of approximately 5.1 billion m^3 in Greece for 2019; see [4]. Additionally, the investment costs and variable costs are chosen such that the sum of the latter corresponds to 6.5% of the market volume.

6.2 Computational setup

All optimization problems have been implemented in Python 3 using Pyomo 5.6.8, see [18], and have been solved with Gurobi 9.0.1, see [16]. In doing so, we used Gurobi with standard settings except for the following adaptions. We set the parameter NumericFocus to 3 and the parameter NonConvex to 2. Thus, Gurobi tackles the nonlinear bilinear terms of Constraint (4c) by spatial branching. For the computations, we used the Kaby Lake nodes with Xeon E3-1240 v6 CPUs and 32 GB RAM of the computer cluster [27] and set a time limit of 24 h. The necessary big-Ms are computed as presented in Sects. 3.1 and 4. Additionally, we used the upper flow bounds of the GasLib 134 network to tighten these big-Ms.

We now briefly discuss some statistics of the considered model. Our single-level model consists of 3599 variables, which contain 698 binary variables, and of 22 085 constraints, which contain 267 quadratic constraints. The presolve of Gurobi roughly halves the number of constraints but hardly influences the other statistics including the number of quadratic constraints. We note that before presolve we have 266 combinatorial constraints (27). In the next section, we discuss the numerical results in detail and explicitly analyze the computational speed up of the combinatorial constraints.

6.3 Discussion of numerical results

The scope of this section is twofold: We first discuss the numerical results w.r.t. running times. Here, we focus on the computational benefit of the combinatorial constraints (27) of Sect. 5. Afterward, we exemplarily show the effects of modifying the economic data on the output of the four-level gas market model for the Greek gas network to shed some light on the sensitivity of the model and the solution approach.

For our discussion of the computational results, we consider 110 instances as described in Sect. 6.1. The running times are summarized in Table 2. Overall, we can solve 107 out of 110 instances to global optimality for the considered four-level gas market model within the time limit. More specifically, we solve 90 of the 110 instances within 1 h. One of the key components to achieve this performance is our modeling of the adjustable robust constraints (4d) and the additional combinatorial constraints (27). The running times significantly increase if these combinatorial constraints are excluded; see Table 2. This leads to the results that 23 instances could not be solved in the time limit of 24 h if the additional combinatorial constraints are neglected. The significant computational speed up of these constraints is underlined by the fact that the minimum running times without them is larger than the median, receptively nearly equal to the third quartile, of the running times including these constraints. Moreover, only 4 of the 110 instances can be solved in 1 h if the additional constraints are excluded.

We further analyze the computational benefit of the combinatorial constraints with the help of log-scaled performance profiles as proposed in [6]. Figure 1 shows the log-scaled performance profiles w.r.t. running times (left) and w.r.t. nodes explored in the branch-and-bound algorithm of Gurobi (right) for all 110 instances. To do so, we separately solved the considered model with the combinatorial constraints (27) and without them. In line with Table 2, the left profile shows that including the combinatorial constraints clearly dominates

Table 2 Number of solved instances (out of 110 instances) and statistics for the running times (always taken only for all instances solved to optimality)

No. of solved	Comb-cons 107	w/o comb-cons 87
	Time (s)	Time (s)
Minimum	251.65	2069.42
1st Quartile	670.65	9790.43
Median	1070.32	17685.29
Mean	2868.59	26193.49
3rd Quartile	2127.64	41813.73
Maximum	32833.46	83639.78

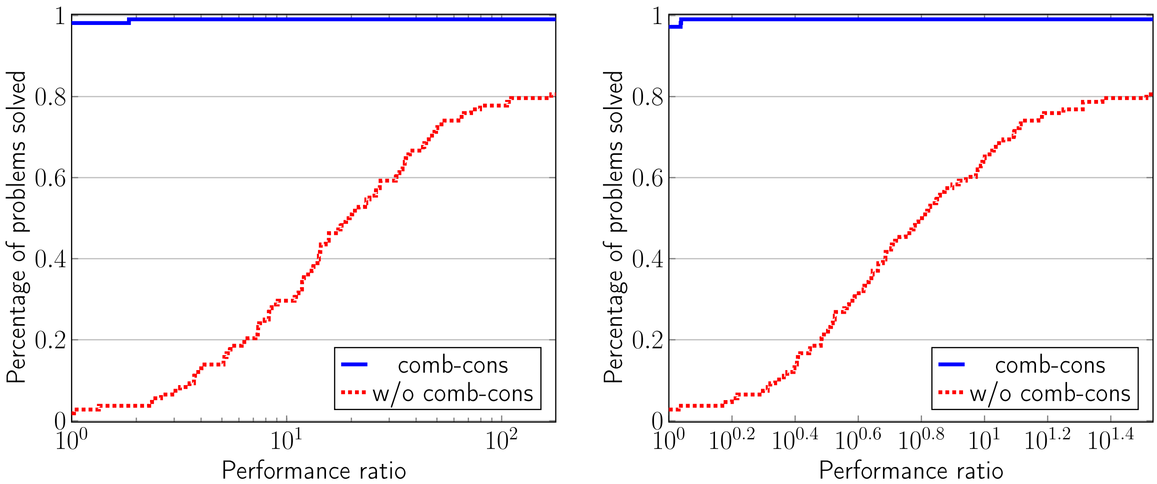

Fig. 1 Log-scaled performance profiles of running times (left) and of nodes explored in the branch and bound algorithm (right) for all 110 instances

w.r.t. running times. This is mainly explained by the right performance profile in Fig. 1, which compares the number of nodes that are explored during the branch-and-bound solution process. Including the combinatorial constraints significantly reduces the number of explored nodes, which leads to the observed speed up of the solution process.

Finally, we now turn to the analysis of the sensitivity of the approach w.r.t. changes in the economic input data. To this end, we consider a base instance with fixed exogenous investment costs $C = 15\,000$€ and variable transport costs $c^{\text{var}} = 0.5$€/bar^2. Then, we adjust the intercepts of the demand functions $a_{i,t}$ for all $i \in \mathcal{P}_u,\ u \in V,\ t \in T$, by adding a constant, which we call "shift". Table 3 shows that increasing, respectively decreasing, the demand mainly affects the nominated amount of gas in the summer period ($t = 0$). The remaining time periods are only slightly affected by demand changes. Moreover, a decrease of the demand affects the nominations more than an increase of the demand. On the one hand, this indicates that for time periods $t \in \{1, 2, 3\}$ the network already operates near to its maximal capacity since an increased demand only slightly leads to higher nominations. On the other hand, the demand in time periods $t \in \{1, 2, 3\}$, especially the winter period $t = 2$, is nearly inelastic since an decrease of the demand only leads to a small decrease of the nominated amount of gas. Moreover, the sum of all booked capacities is nearly the same. This can be explained by the almost inelastic demand of the winter period since, usually, the booking is determined by the period with highest demand, i.e., it is determined in winter. Although the total booked capacity is almost not affected by the change of the demand, the

Table 3 For all $i \in \mathcal{P}_u$, u, $t \in T$, the intercepts $a_{i,t}$ vary by adding "shift" in €/(1000 Nm^3/h). The remaining values denote the corresponding relative changes of the bookings q^{book}, and nominations q^{nom} w.r.t. the base case marked in bold

shift	$\frac{\|q^{\text{book}}\|_1}{\|q^{\text{book}}_{\text{base}}\|_1}$	$\frac{q^{\text{book}}_v}{q^{\text{book}}_{\text{base},v}}$ in ...	$\frac{\|q^{\text{nom}}_0\|_1}{\|q^{\text{nom}}_{\text{base},0}\|_1}$	$\frac{\|q^{\text{nom}}_1\|_1}{\|q^{\text{nom}}_{\text{base},1}\|_1}$	$\frac{\|q^{\text{nom}}_2\|_1}{\|q^{\text{nom}}_{\text{base},2}\|_1}$	$\frac{\|q^{\text{nom}}_3\|_1}{\|q^{\text{nom}}_{\text{base},3}\|_1}$
−10	0.99	[0.88, 1.20]	0.42	0.90	1.00	0.86
−5	1.00	[0.93, 1.12]	0.71	0.97	1.00	0.96
0	**1.00**	**[1.00, 1.00]**	**1.00**	**1.00**	**1.00**	**1.00**
5	1.01	[0.97, 1.08]	1.18	1.01	1.01	1.02
10	1.01	[0.95, 1.13]	1.24	1.02	1.01	1.02

booked capacity at the single nodes clearly differs; see third column of Table 3. Thus, the overall solution of the four-level optimization problem is clearly affected by demand changes; see Table 3. We illustrate these changes w.r.t. the bookings in Fig. 2. The figure shows that uniformly increasing the demand of all exits decreases the booked capacities in the south and leads to larger booked capacities in the middle, respectively north, of the network. This is possibly based on a combination of the larger willingness to pay of the exits and the transport capacity of the network. There are more exits in the south than in the north and, thus, the network probably already operates at its maximum especially in the south. Consequently, an increased willingness to pay at the demand nodes makes it more attractive for the TSO to reduce the technical capacities in the south and increase them in the north. This results in larger bookings in the north and smaller bookings in the south.

7 Conclusion

This paper provides optimization techniques that enable us to solve a multilevel model of the European entry-exit gas market system, see [14], with a nonlinear flow model for real-world sized and tree-shaped networks. In line with the literature [2,14], this multilevel model can be equivalently reformulated to a bilevel problem and, on top of that, to a nonconvex and nonsmooth mixed-integer nonlinear single-level problem. This reformulation is independent of the considered flow model. The core difficulty of this single-level reformulation are the nonlinear adjustable robust constraints, by which the TSO computes the technical capacities of the network. These constraints alone make the considered problem computationally intractable in general. However, under the assumption of passive networks, i.e., no active elements such as compressor stations are considered, we derived a finite-dimensional reformulation of these nonlinear adjustable robust constraints for the case of tree-shaped networks. Moreover, we strengthened this reformulation by additional combinatorial constraints. The latter significantly increase the performance of our model as demonstrated by the numerical results. Further, the presented reformulation can also be generalized to other potential-based flow models under very mild assumptions. The reformulation has some nice properties such that it only uses convex constraints including newly introduced integer variables. This enables us to solve the multilevel model of the European entry-exit gas market system with a nonlinear flow model for a real-world sized network, namely the Greek gas network without active elements, to global optimality. This is the first time that this multilevel model can be solved for a real-world sized network since even for simplified linear flow models the

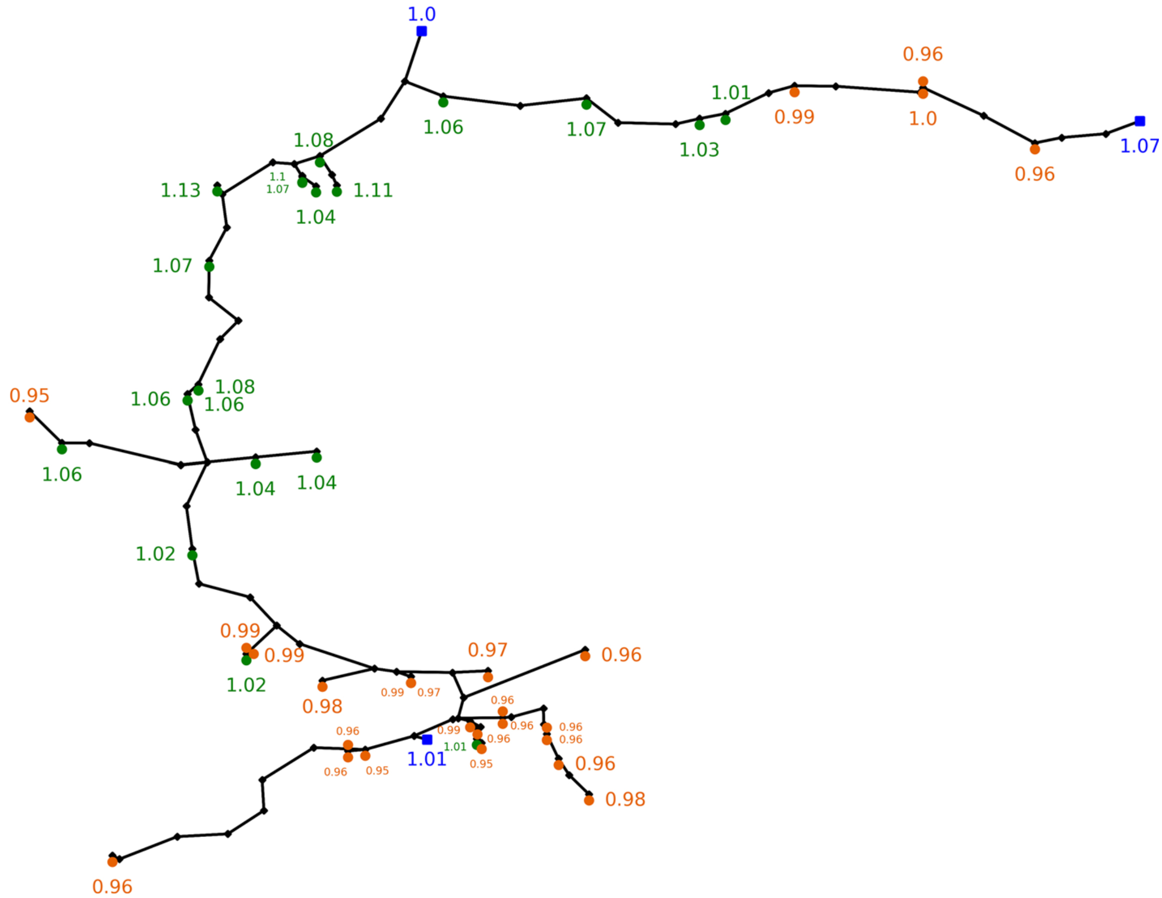

Fig. 2 Relative changes of the bookings, i.e., $q_v^{\text{book}}/q_{\text{base},v}^{\text{book}}$, for the case shift $= 10$ and the base case (shift $= 0$) in the Greek gas network. Entries are denoted by blue squares, inner nodes by small black diamonds, exits with positive relative change by green circles, and exits with negative relative change by orange circles

latter can only be solved for stylized small (but cyclic) networks so far in the literature. The computational tractability of our approach is demonstrated by our computational study, in which the majority of the instances can be solved within 1 h.

Nevertheless, there still are many possibilities for future research. Both from a mathematical as well as application point of view, it would be of interest to see if the results can be further developed so that one can also cope with active elements or general, i.e., cyclic, networks. From an economic point of view, our results can be directly applied to analyze economic effects such as social welfare losses for real-world sized networks and nonlinear flow models.

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