When Bilevel Optimization Meets Gas Networks: Feasibility of Bookings in the European Entry-Exit Gas Market

Computational Complexity Results and Bilevel Optimization Approaches

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Acknowledgments

Almost four years ago, I started my PhD in optimization as a member of the "Graphs and Mathematical Optimization" research group at Université libre de Bruxelles. At that time, I was blissfully unaware of the challenges it entailed and all the fascinating people I would meet over the years. Now, amid the COVID-19 pandemic, this exciting chapter comes to an end with a dissertation submitted for a joint PhD degree between Université libre de Bruxelles and Universität Trier. It goes without saying that I would not be where I am today without the support of a lot of people. In a first place, I would like to thank all three of my supervisors.

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Abstract

Transport and trade of gas are decoupled after the liberalization of the European gas markets, which are now organized as so-called entry-exit systems. At the core of this market system are bookings and nominations, two special capacity-right contracts that grant traders access to the gas network. The latter is operated by a separate entity, known as the transmission system operator (TSO), who is in charge of the transport of gas from entry to exit nodes. In the mid to long term, traders sign a booking contract with the TSO to obtain injection and withdrawal capacities at entry and exit nodes, respectively. On a day-ahead basis, they then nominate within these booked capacities a balanced load flow of the planned amounts of gas to be injected into and withdrawn from the network the next day. The key property is that by signing a booking contract, the TSO is obliged to guarantee transportability for all balanced load flows in compliance with the booked capacities. To assess the feasibility of a booking, it is therefore necessary to check the feasibility of infinitely many nominations. As a result, deciding if a booking is feasible is a challenging mathematical problem, which we investigate in this dissertation.

Our results range from passive networks, consisting of pipes only, to active networks, containing controllable elements to influence gas flows. Since the study of the latter naturally leads to a bilevel framework, we first consider some more general properties of bilevel optimization. For the case of linear bilevel optimization, we consider the hardness of validating the correctness of big-Ms often used in solving these problems via a single-level reformulation. We also derive a family of valid inequalities to be used in a bilevel-tailored branch-and-cut algorithm as a big-M-free alternative.

We then turn to the study of feasible bookings. First, we present our results on passive networks, for which bilevel approaches are not required. A characterization of feasible bookings on passive networks is derived in terms of a finite set of nominations. While computing these nominations is a difficult task in general, we present polynomial complexity results for the special cases of tree-shaped or single-cycle passive networks. Finally, we consider networks with linearly modeled active elements. After obtaining a bilevel optimization model that allows us to determine the feasibility of a booking in this case, we derive various single-level reformulations to solve the problem. In addition, we obtain novel characterizations of feasible bookings on active networks, which generalize our characterization in the passive case. The performance of these various approaches is compared in a case study on two networks from the literature, one of which is a simplified version of the Greek gas network.

Résumé

Transport et commerce de gaz sont découplés depuis la libéralisation des marchés européens du gaz, qui sont désormais organisés en systèmes dit d'entrée-sortie. Au cœur de ce système de marché se trouvent les réservations et les nominations, deux contrats spéciaux de droit à la capacité qui permettent aux négociants d'accéder au réseau de gaz. Ce dernier est exploité par une entité distincte, appelée gestionnaire de réseau de transport (GRT), qui est chargée du transport du gaz entre les nœuds d'entrée et de sortie. À moyen et long terme, les négociants signent un contrat de réservation avec le GRT pour obtenir des capacités d'injection et d'extraction aux nœuds d'entrée et de sortie, respectivement. Au jour le jour, ils désignent ensuite, dans les limites des capacités réservées, un flux de charge équilibrée des quantités de gaz prévues à injecter et à extraire le lendemain. La propriété essentielle est qu'en signant un contrat de réservation, le GRT est obligé de garantir la transportabilité de tous les flux de charge équilibrée respectant les capacités réservées. Pour évaluer la faisabilité d'une réservation, il est donc nécessaire de vérifier la faisabilité d'une infinité de nominations. Par conséquent, décider si une réservation est réalisable est un problème mathématique difficile, que nous étudions dans cette thèse.

Nos résultats vont des réseaux passifs, constitués uniquement de pipelines, aux réseaux actifs, contenant des éléments contrôlables pour influencer les flux de gaz. Comme l'étude de ces derniers conduit naturellement à un cadre biniveau, nous considérons d'abord certaines propriétés plus générales de l'optimisation biniveau. Pour le cas de l'optimisation biniveau linéaire, nous étudions la difficulté de valider l'exactitude des constantes de type big-M souvent utilisées dans la résolution de ces problèmes via une reformulation à un seul niveau. Nous déduisons également une famille d'inégalités valides à utiliser dans un algorithme de branch-and-cut adapté au biniveau comme alternative à l'approche utilisant des big-Ms.

Nous nous tournons ensuite vers l'étude des réservations réalisables. D'abord, nous présentons nos résultats sur les réseaux passifs, pour lesquels les approches biniveaux ne sont pas nécessaires. Une caractérisation des réservations réalisables sur les réseaux passifs est déduite en termes d'un ensemble fini de nominations. Bien que le calcul de ces nominations soit une tâche difficile en général, nous présentons des algorithmes polynomiaux pour les cas particuliers des réseaux passifs en forme d'arbre ou contenant un cycle unique. Enfin, nous considérons les réseaux avec des éléments actifs modélisés à l'aide de contraintes linéaires. Après avoir obtenu un modèle biniveau, permettant de déterminer la faisabilité d'une réservation dans ce cas, nous dérivons diverses reformulations à un seul niveau pour résoudre le problème. En outre, nous obtenons de nouvelles caractérisations des réservations réalisables sur les réseaux actifs, qui généralisent notre caractérisation dans le cas passif. La performance de ces différentes approches est comparée dans une étude de cas réalisée sur deux réseaux de la littérature, dont l'un est une version simplifiée du réseau de gaz grec.

Zusammenfassung

Nach der Liberalisierung der europäischen Gasmärkte, welche nun als sogenannte Entry-Exit Systeme organisiert sind, sind Transport und Handel von Gas entkoppelt. Im Zentrum dieses neuen Marktsystems sind Buchungen und Nominierungen, zwei spezielle Kapazitätrechtsverträge, die Händlern Zugang zum Gasnetz gewähren. Letzteres wird von einem separaten Akteur betrieben, dem sogenannten Fernleitungsnetzbetreiber (FNB), der für den Transport des Gases von den Einspeise- zu den Ausspeiseknoten verantwortlich ist. Händler schließen mittel- bis langfristig einen Buchungsvertrag mit dem FNB ab, um Ein- und Ausspeisekapazitäten zu erhalten. Täglich nominieren sie dann innerhalb der gebuchten Kapazitäten einen bilanzierten Lastfluss der geplanten Gasmengen, die am nächsten Tag eingespeist und entnommen werden sollen. Die Haupteigenschaft ist, dass der FNB sich durch Unterzeichnung eines Buchungsvertrages für die Transportierbarkeit aller bilanzierten Lastflüsse innerhalb der gebuchten Kapazitäten verpflichtet. Um die Zulässigkeit einer Buchung zu bestimmen ist es daher notwendig, die Zulässigkeit von unendlich vielen Nominierungen zu prüfen. Die Entscheidung, ob eine Buchung zulässig ist, ist daher ein anspruchsvolles mathematisches Problem, das wir in dieser Dissertation untersuchen.

Unsere Ergebnisse reichen von passiven Netzen, die nur aus Rohren bestehen, bis hin zu aktiven Netzen, die steuerbare Elemente zur Beeinflussung der Gasflüsse enthalten. Da die Untersuchung aktiver Netze uns auf natürlichem Wege zu Bilevel-Problemen führt, betrachten wir zunächst einige allgemeinere Eigenschaften der Bilevel-Optimierung. Für den Fall der linearen Bilevel-Optimierung betrachten wir die Schwierigkeit, Big-Ms zu validieren, die oft bei der Lösung dieser Probleme mittels einer einstufigen Reformulierung verwendet werden. Wir leiten außerdem eine Familie gültiger Ungleichungen ab, die in einem Bilevel-spezifischen Branch-and-Cut Algorithmus als big-M-freie Alternative verwendet werden können.

Wir wenden uns dann der Untersuchung von zulässigen Buchungen zu. Zunächst stellen wir unsere Ergebnisse zu passiven Netzwerken vor, für die Bilevel-Ansätze nicht erforderlich sind. Eine Charakterisierung zulässiger Buchungen in passiven Netzwerken wird in Bezug auf eine endliche Menge an Nominierungen hergeleitet. Während die Berechnung dieser Nominierungen im Allgemeinen eine schwierige Aufgabe ist, präsentieren wir polynomielle Komplexitätsergebnisse für die Spezialfälle baumförmiger oder einzyklischer passiver Netze. Schließlich betrachten wir Netze mit linear modellierten aktiven Elementen. Nachdem wir ein Bilevel-Modell hergeleitet haben, mit dem wir die Zulässigkeit einer Buchung in diesem Fall bestimmen können, leiten wir verschiedene einstufige Reformulierungen zur Lösung des Problems ab. Darüber hinaus erhalten wir neuartige Charakterisierungen zulässiger Buchungen auf aktiven Netzen, die unsere Charakterisierung im passiven Fall verallgemeinern. Die Anwendbarkeit dieser verschiedenen Ansätze wird in einer Fallstudie an zwei Netzen aus der Literatur verglichen, wovon eines eine vereinfachte Version des griechischen Gasnetzes ist.

Author's Contributions

The present dissertation is the result of a collection of peer-reviewed journal articles as well as submitted preprints. Part I is an extended summary of the ideas and results contained in these works. Their contributions are situated within the literature and the links between the different publications are discussed. Part II is a collection of reprints of published journal articles and submitted preprints. Since all of these works have been the result of on-going scientific collaborations with different co-authors, the contributions of the author of this dissertation are clearly stated in the following.

[FP1] Kleinert, T., M. Labbé, F. Plein, and M. Schmidt (2020). "Technical Note—There's No Free Lunch: On the Hardness of Choosing a Correct Big-M in Bilevel Optimization." In: *Operations Research* 68.6, pp. 1716–1721. DOI: 10.1287/opre.2019.1944.

The main ideas for this article are the result of joint discussions of all four authors. All proofs have been developed by Fränk Plein and he contributed to the writing of the paper.

[FP2] Kleinert, T., M. Labbé, F. Plein, and M. Schmidt (2021). "Closing the Gap in Linear Bilevel Optimization: A New Valid Primal-Dual Inequality." In: *Optimization Letters* 15.4, pp. 1027–1040. DOI: 10.1007/s11590-020-01660-6.

The derivation of the valid inequalities was the consequence of joint discussions of all four authors of the article. Fränk Plein was the primary contributor for the implementation of the solution approach. Additionally, he was the primary author of the fourth section.

[FP3] Labbé, M., F. Plein, and M. Schmidt (2020). "Bookings in the European Gas Market: Characterisation of Feasibility and Computational Complexity Results." In: *Optimization and Engineering* 21.1, pp. 305–334. DOI: 10.1007/s11081-019-09447-0.

Fränk Plein contributed ideas and proofs for the results in this article. He was the primary author of the paper, in close discussion with the other authors.

[FP4] Labbé, M., F. Plein, M. Schmidt, and J. Thürauf (2021). "Deciding Feasibility of a Booking in the European Gas Market on a Cycle is in P for the Case of Passive Networks." In: *Networks*. 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. Fränk Plein contributed theoretical results and proofs that finally led to the main result of this paper. Fränk Plein was one of the primary authors of the article.

[FP5] Plein, F., J. Thürauf, M. Labbé, and M. Schmidt (2021). *A Bilevel Optimization Approach to Decide the Feasibility of Bookings in the European Gas Market*. Preprint. Submitted. URL: http://hdl.handle.net/2013/ULB-DIPOT:oai:dipot.ulb.ac.be:2013/318633.

The idea to study the feasibility of bookings on networks 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. He also contributed significant parts in the writing of the article.

Finally, the following peer-reviewed article has been co-authored by the author of this dissertation during his doctoral studies. Since this article is a direct follow-up of his Master's thesis and since the research therein is concerned with a different topic, it has been omitted from this dissertation.

[FP6] Bucarey, V., S. Elloumi, M. Labbé, and F. Plein (2021). "Models and algorithms for the product pricing with single-minded customers requesting bundles." In: *Computers & Operations Research* 127, pp. 105–139. DOI: 10.1016/j.cor.2020.105139.

Contents

Part I

Extended Summary

1

Introduction

The European Commission (2018) presented eight scenarios to achieve the goal set out in the European Green Deal (European Commission 2019), i.e., a carbon-neutral energy system in 2050. In all of these scenarios, gas plays a key role. Natural gas is transported through large pipeline networks, with long-distance transmission systems in the European Union and the United Kingdom having a combined length of around 198 500 km in 2020 (ENTSOG 2020). In addition, there are distribution systems operated on a smaller scale to ship gas to the end-customers, resulting, e.g., in Germany alone, in a total network length of over 500 000 km of pipelines (Federal Ministry for Economic Affairs and Energy 2017). In this work, we only consider problems that mostly arise on European transmission systems and therefore focus on this type of networks.

With the continuing rise of the share of renewable resources in the overall energy mix, existing gas infrastructure attracts an increasing interest to hedge against energy-supply uncertainties. The compressibility of gas and the recent development and study of power-to-gas technologies allow to use gas networks for additional transport routes and, more notably, as storage for excess renewable energies; see, e.g., Jentsch et al. (2014). This added flexibility can support the shift away from fossil fuels towards renewable energy resources. It enables novel possibilities to store the excess of energy produced in periods of high supply to then cover the demand in periods of lower supply. We refer to the review by Götz et al. (2016) for technological and economic aspects of power-to-gas in general and the review by Wulf et al. (2018) for recent European research and demonstration projects. While the consumption of natural gas has a smaller carbon footprint compared to equivalent amounts of oil or coal, it is still a fossil fuel. The European Commission (2020) discusses the benefits of so-called renewable hydrogen as an alternative and clean fuel. Although hydrogen is more flammable than natural gas, existing transmission systems could be repurposed; see, e.g., Dodds and Demoullin (2013) and Siemens Energy et al. (2020). However, hydrogen is already blended into natural gas networks in smaller percentages. Melaina et al. (2013) discuss some of the key issues on the example of networks in the United States. De Vries et al. (2017) study the interchangeability of natural gas and hydrogen mixtures with respect to (w.r.t.) end-use equipment. Altogether, these novel use cases of gas networks have given rise to a vast stream of literature on integrated gas and electricity systems in Europe and beyond; see, e.g., Alabdulwahab et al. (2015), Bent et al. (2018), Biskas et al. (2016), Borraz-Sanchez et al. (2016), Byeon and Hentenryck (2020), Chen et al. (2018), Clegg and Mancarella (2015), Correa-Posada and Sanchez-Martin (2015), Gil et al. (2016), Li et al. (2017), Ordoudis et al. (2017), Schwele et al. (2019), Zhao et al. (2017), and Zlotnik et al. (2017). The accurate assessment of capacities of existing gas networks thus becomes a crucial task in an evolving European energy system.

1.1 Liberalization of European Gas Markets

Since the 1990s, the European Union has undertaken ongoing efforts to liberalize its gas markets; see the Directives and Regulations of the European Parliament and Council of the European Union (1998, 2003, 2005, 2009a,b). The decoupling of gas transport and trade has led to the adoption of the so-called entry-exit market system; see, e.g., Hewicker and Kesting (2009) and Grimm et al. (2019). In this market organization, the network is controlled by the transmission system operator (TSO). Gas traders access the network via special capacity-right contracts to get gas shipped from entry to exit points. First, traders sign a booking contract with the TSO, which specifies an upper bound on the amount of gas to be injected into or withdrawn from the network at entry or exit nodes. On a day-ahead basis, traders then nominate a balanced load flow specifying the planned amount of gas to be transported through the network the next day. By signing a booking contract, the TSO is legally obliged to guarantee the transportability of every balanced nomination within the booked capacities. A booking is therefore said to be feasible if all booking-compliant nominations, i.e., infinitely many, can be transported. In this dissertation, we will show that deciding the feasibility of a booking is a challenging mathematical task.

1.2 Feasibility of Nominations

The dynamics of gas flow are governed by partial differential equations; see, e.g., Hante et al. (2017) and the PhD thesis by Sirvent (2018). In this dissertation, we only consider stationary gas flows. In this case, Groß et al. (2019) discuss that gas physics can be approximated by algebraic equations; see also the book edited by Koch et al. (2015). A lot of research considers the feasibility of nominations, i.e., the possibility to transport a given load flow within the technical restrictions of the network, as well as its cost-optimal transport. In the early work by Wong and Larson (1968), dynamic programming is applied to optimize gas transport. Further early studies analyze physical properties of gas networks. Maugis (1977) and Collins et al. (1978) show that gas flows in pipeline networks are uniquely determined by the load flow and that they are the solution of a strictly convex minimization problem. As a consequence of the liberalization of gas markets, there has been a significant increase in studies applying mathematical optimization in the gas sector starting in the early 2000s. Ríos-Mercado et al. (2002) study reduction techniques for complex gas networks by investigating which decision variables can be fixed a priori. On the example of the Belgian network, De Wolf and Smeers (2000) and Bakhouya and De Wolf (2007) study the cost-optimal transport of gas before and after the liberalization. The authors propose an adaptation of the simplex algorithm for the case in which gas physics are approximated by piecewise-linear functions. As an extension, piecewise-linear relaxations for gas physics are studied by Geißler et al. (2015a,b, 2018) and in the PhD thesis by Geißler (2011). A variety of techniques for checking the feasibility of a nomination are presented by Pfetsch et al. (2014) and in the book edited by Koch et al. (2015). Besides piecewise-linear approximations and relaxations, the problem is tackled via nonlinear programming approaches by Gollmer et al. (2015) and Schmidt et al. (2013, 2015b, 2016). Techniques from mathematical programming with equilibrium constraints are applied by Baumrucker and Biegler (2010), Schmidt et al. (2015a), and Rose et al. (2016) and in the PhD thesis by Schmidt (2013). The combination of nonlinear gas physics and discrete decision variables for controlling the network quickly leads to challenging mixed-integer nonlinear problems (MINLPs), as observed in the works by Geißler et al. (2013), Humpola et al. (2015), Rose et al. (2016), and Geißler et al. (2018) or the PhD thesis by Morsi (2013). The high interest in problems of gas transport has also led to the creation of the GasLib (Schmidt et al. 2017), a collection of networks and historical nomination data inspired by real-life networks such as the Greek transmission network. The GasLib also contains important test cases relevant in many previously cited works. Borraz-Sánchez et al. (2016) study mixed-integer second-order cone relaxations of gas flows for network expansion planning and assess their methods for an expansion of the Belgian network. For a more general overview of challenging mathematical problems in gas networks, we refer to the survey by Ríos-Mercado and Borraz-Sánchez (2015) and the references therein.

1.3 Feasibility of Bookings

In contrast, the literature on the feasibility of bookings is much sparser. First analyses of bookings date back to the technical report by Szabó (2012) as well as the PhD thesis by Willert (2014). In another early technical report by Fügenschuh et al. (2014), the reservation-allocation problem is studied, which is closely related to the feasibility of a booking. Hayn et al. (2015) present first efforts to verify booked capacities heuristically using tools from stochastic optimization. In the PhD thesis by Hayn (2017), the computational complexity of checking the feasibility of a booking is studied and first exact solution approaches using semi-algebraic sets are presented. Schewe et al. (2020c) establish structural properties of the sets of feasible nominations and bookings such as nonconvexity and star-shapedness.

Deciding the feasibility of a booking can be seen as an adjustable, respectively two-stage, robust feasibility problem with uncertain load flows. In this view, the uncertainty set contains all booking-compliant nominations and all variables are "wait-and-see" decisions, since the gas transport is only determined once a nomination is given. For an overview of adjustable robust optimization, we refer to the book by Ben-Tal et al. (2009) and the survey by Yanıkoğlu et al. (2019). Aßmann et al. (2018, 2019) develop techniques for particular two-stage robust optimization problems and illustrate their effectiveness on the example of gas networks. Their results are also found in the PhD thesis by Aßmann (2019). Kuchlbauer et al. (2020) present bundle methods for nonlinear robust optimization using the example of gas transport. The problem of robustly selecting pipe diameters under load flow uncertainties is studied by Robinius et al. (2019). In the setting with uncertain withdrawals, Vuffray et al. (2015) exploit monotonicity properties of gas flows to solve a robust maximum profit problem more effectively.

1.4 Bilevel Optimization in Energy Networks and Markets

Two-stage robust optimization problems with an empty first stage can be recast as bilevel problems by letting one player control the uncertainties and another the "wait-and-see" decision variables. Historically, the first studies related to bilevel optimization date back to the works of von Stackelberg (1934) on leader-follower games, in which two players interact successively. Bilevel problems are mathematical optimization problems in which a subset of variables is constrained to be the solution of another optimization problem. A first formal definition of bilevel problems in operations research is given by Bracken and McGill (1973) for a military application. The formulation introduced therein is commonly used in the present-day literature. Another early discussion by Candler and Norton (1977) also considers bilevel problems and, more generally, multilevel optimization. After the 1970s, bilevel optimization attracted a serious interest in the literature for its capability to model hierarchical decision processes; see Anandalingam and Friesz (1992). A lot of early efforts are devoted to linear bilevel optimization, as shown in the surveys by Wen and Hsu (1991), Ben-Ayed (1993), and Vicente and Calamai (1994). For a general overview of bilevel optimization, we refer to the surveys by Colson et al. (2005) and Colson et al. (2007) as well as the books by Bard (1998) and Dempe (2002). The recent survey by Kleinert et al. (2021a) reviews mixed-integer techniques that are often applied to solve bilevel problems. Finally, the book edited by Dempe and Zemkoho (2020) contains many recent advances and future challenges in bilevel optimization, including a very detailed bibliography of bilevel optimization by Dempe (2020).

The book by Gabriel et al. (2013) shows that bilevel optimization has proven to be a suitable tool to model adversarial interactions often encountered in problems related to energy networks and markets in general. A lot of research considers network expansion problems in market environments; see, e.g., Fan and Cheng (2009), Garces et al. (2009), Garcia-Herreros et al. (2016), and Bylling et al. (2020). On the other hand, bilevel optimization is often considered to model and study aspects of energy markets. We refer to the recent survey by Wogrin et al. (2020) for an overview. Besides electricity networks and markets, bilevel optimization is also applied in the gas sector. Dempe et al. (2005, 2011) and Kalashnikov et al. (2010) apply techniques from discrete bilevel optimization to tackle the natural gas cash-out problem. Hennig and Schwarz (2016) use bilevel optimization to detect severe transport situations in gas networks. A multilevel model of the European entry-exit gas market is presented by Grimm et al. (2019) and the authors show that it can be equivalently reformulated with two levels. Based on this bilevel reformulation, Böttger et al. (2020) study the cost of decoupling and inefficiencies due to the market organization after liberalization. Similarly, Schewe et al. (2020b) present algorithms to solve the model by Grimm et al. (2019) on the example of the Greek gas network. Very recently, the European gas market is studied by Heitsch et al. (2021) with added chance constraints to take into account uncertain load flows.

1.5 Contribution and Structure

The contribution of this dissertation is twofold and lies at the intersection of bilevel optimization and the study of the European entry-exit gas market. One of the goals of the research encapsulated in this PhD thesis is to convey a better understanding of the problem of deciding the feasibility of bookings in the entry-exit market system. At first, we consider passive networks, i.e., networks that do not contain controllable elements such as compressors or control valves. In this case, single-level formulations are sufficient to represent the problem. In [FP3], we present a characterization of feasible bookings on passive networks, determined by bounds on the optimal solutions of nonlinear and nonconvex maximization problems. We also show that these problems can be solved in polynomial time on passive tree-shaped networks. As a next step, we investigate the problem on a single passive cycle in [FP4]. For this case, after an extensive analysis of the optimal solutions involved in the characterization of feasible bookings, we show that the feasibility of a booking can still be checked in polynomial time. To this end, we combine our structural insights with tools from real algebraic geometry to derive a polynomial-time algorithm.

In contrast to passive networks, deciding the feasibility of a booking on active networks naturally leads to a bilevel framework. Consequently, we consider relevant aspects when solving bilevel problems via a single-level reformulation. For the case of linear bilevel optimization, we investigate in [FP1] the hardness of validating big-Ms necessary for the linearization of a single-level reformulation commonly found in the bilevel literature. As a direct follow-up, we develop valid inequalities in [FP2] to be used in a big-M-free branch-and-cut approach for linear bilevel optimization.

Finally, we apply techniques from bilevel optimization in our study of the European gas market in [FP5]. Therein, we consider the feasibility of a booking on networks with linearly modeled active elements. We first show that the characterization for passive networks in [FP3] cannot be applied anymore. We model the feasibility of a booking as a bilevel problem, taking into account the influence the TSO has on gas flows by controlling the active elements in the network. Various single-level reformulations are presented and novel characterizations of feasible bookings are derived that generalize the result in [FP3].

The remainder of Part I of this dissertation is structured as follows. In Chapter 2, we introduce basic notations and results of bilevel optimization and present the main results of [FP1; FP2]. Chapter 3 is devoted to the modeling of gas transport in the European entry-exit market. Therein, besides the foundations of gas physics and the approximation studied in this dissertation, we also give formal definitions of nominations and bookings in the entry-exit system and review results from the literature that are closely related to our work. In Chapter 4, we then present the findings of [FP3; FP4] w.r.t. passive networks, before turning to our study of active networks in [FP5] using tools from bilevel optimization. Finally, we draw some conclusions in Chapter 5, where we also discuss remaining challenges and future research.

2

Bilevel Optimization

In this chapter, we discuss basic notions of bilevel optimization as well as novel results. In Section 2.1, we introduce the notations of bilevel optimization used in the following. We then turn to classic reformulation techniques in Section 2.2 to rephrase bilevel problems as single-level optimization problems. In Section 2.3, challenges of bilevel optimization and some solution approaches for the single-level reformulations are discussed. For these first three sections, we mainly follow the presentation of the books by Bard (1998) and Dempe (2002). In the remaining two sections, we present novel results from [FP1; FP2] for linear bilevel problems. In Section 2.4, we discuss the challenges of finding correct big-Ms for the linearization of a well-known single-level reformulation. Finally, in Section 2.5, we present a new family of valid inequalities to be used in a big-M-free branch-and-cut framework.

2.1 Notation

In bilevel optimization, one models the successive interaction of two players. The first player, called the *leader*, takes a decision $x \in \mathbb{R}^k$ to optimize a given objective function, while anticipating the optimal reaction of the second player. The latter, called the *follower*, then reacts optimally with $y \in \mathbb{R}^l$ dependent on the leader's decision x. Let the leader's objective function $F : \mathbb{R}^k \times \mathbb{R}^l \to \mathbb{R}$, the follower's objective function $f : \mathbb{R}^k \times \mathbb{R}^l \to \mathbb{R}$, and constraint functions $G : \mathbb{R}^k \times \mathbb{R}^l \to \mathbb{R}^m$ and $g : \mathbb{R}^k \times \mathbb{R}^l \to \mathbb{R}^n$ be given. Furthermore, let $X \subseteq \mathbb{R}^k$ and $Y \subseteq \mathbb{R}^l$ denote two sets encoding additional constraints on leader and follower variables, such as bounds or integrality constraints on a subset of variables. The bilevel problem is then formally defined by

$$\max_{x \in X} \quad F(x, y) \quad \text{s.t.} \quad G(x, y) \leq 0, \ y \in \mathcal{S}(x), \tag{2.1}$$

where $\mathcal{S}(x)$ contains the optimal solutions of the parametric optimization problem with parameter x, given by

$$\min_{y \in Y} \quad f(x,y) \quad \text{s.t.} \quad g(x,y) \geq 0. \tag{2.2}$$

The *upper-level* or *leader problem* is given by (2.1), whereas the inner optimization problem (2.2) defines the *lower-level* or *follower problem.* The set $\mathcal{S}(x)$ contains the follower's optimal reactions to the leader's decision x. It is sometimes referred to as the follower's *rational reaction set.* Upper-level constraints $G(x,y) \leq 0$ are *coupling constraints* if they depend on lower-level variables y. The upper-level variables x that appear in the lower level are known as *linking variables.* Note that the use of "max" in (2.1) is only adequate if the optimal solution is attained. In the presence of integer variables at the lower level, continuous linking variables may lead to unattainable bilevel solutions; see, e.g., Moore and Bard (1990), Vicente et al. (1996), and Köppe et al. (2010). In this thesis, we only consider problems for which the optimal solution is attained and thus refrain from the more general use of "sup", except where explicitly discussed in [FP5] and Section 4.4.

We denote the shared constraint set of Problem (2.1) by

$$\Omega := \{(x,y) \in X \times Y \colon G(x,y) \leq 0,\ g(x,y) \geq 0\}.$$

In order to guarantee that Problem (2.1) is feasible and bounded, it is often assumed that Ω is nonempty and compact. Let Ω_x be the projection of Ω onto the upper-level decisions x, i.e., $x \in \Omega_x$ if there exists y such that $(x,y) \in \Omega$. Then, Ω_x denotes the set of upper-level decisions for which the lower-level problem is feasible. The set of *bilevel-feasible points*, the so-called *inducible region*, is given by

$$\mathrm{IR} := \{(x,y) \in \Omega \colon y \in \mathcal{S}(x)\}.$$

The leader anticipates the follower's rational reaction. In general, the lower-level optimal solution is, however, not uniquely determined, i.e., the rational reaction set is not a singleton. Thus, Problem (2.1) has some ambiguity in the selection of the lower-level decision $y \in \mathcal{S}(x)$. Different approaches can be considered to resolve this ambiguity and determine the choice of the lower-level solution. The *optimistic approach* selects the lower-level solution that is most in favor of the upper level, so that Problem (2.1) becomes

$$\max_{x,y} \quad F(x,y) \quad \text{s.t.} \quad G(x,y) \leq 0,\ x \in X,\ y \in \mathcal{S}(x). \tag{2.3}$$

The *pessimistic approach*, on the contrary, assumes that the follower reacts in a way that is the worst possible for the leader. In this dissertation, whenever the lower-level solution is not uniquely determined, we only study the optimistic approach and refer to Wiesemann et al. (2013) for an overview of pessimistic bilevel optimization.

The difficulty of bilevel optimization lies in the definition of the inducible region, which is defined via the optimality of the lower level. By omitting the constraint on the optimality of the follower's reaction, i.e., $y \in \mathcal{S}(x)$, we obtain a relaxation of (2.1) often found in the literature and referred to as the *high-point relaxation*. It is given by

$$\max_{x,y} \quad F(x,y) \quad \text{s.t.} \quad (x,y) \in \Omega. \tag{2.4}$$

If Ω is not assumed bounded, the high-point relaxation value might be unbounded. In this case, it is shown in Xu (2012) and Xu and Wang (2014) that the bilevel problem can still be infeasible, unbounded, or admit a finite-valued solution. The unboundedness of the high-point relaxation does therefore not allow to infer the unboundedness of the bilevel problem.

According to the nature of the follower's objective and constraint functions, different optimality conditions can be added to (2.4) to ensure that $y \in \mathcal{S}(x)$ for any upper-level decision $x \in \Omega_x$. In the next section, we study reformulations of Problem (2.1) as a single-level optimization problem, while emphasizing the case of a linear lower level.

2.2 Single-Level Reformulations

A first single-level reformulation is obtained by means of the lower-level *optimal value function* given by

$$\varphi(x) := \min_{y \in Y} \{f(x,y) \colon g(x,y) \geq 0\}.$$

Problem (2.1) can equivalently be written as

$$\max_{x,y} \quad F(x,y) \quad \text{s.t.} \quad (x,y) \in \Omega, \; f(x,y) \leq \varphi(x). \tag{2.5}$$

Only points $(x,y) \in \Omega$ that have a value $f(x,y)$ not larger than the corresponding lower-level optimal value $\varphi(x)$ are considered, which ensures that $y \in \mathcal{S}(x)$. Note that by optimizing the leader's objective function over both the leader and follower variables, Problem (2.5) leads to the optimistic approach (2.3). The same holds for all reformulations presented in the following.

In the remainder of this section, we focus on bilevel problems, in which the lower level is a linear program (LP) in both x and y. We thus assume that f and g are linear functions and that Y is a polyhedron. In this case, the rational reaction set $\mathcal{S}(x)$ contains the optimal solutions of

$$\min_{y} \quad f^\top y \quad \text{s.t.} \quad Cx + Dy \geq b, \tag{2.6}$$

with $f \in \mathbb{R}^l$, $C \in \mathbb{R}^{n \times k}$, $D \in \mathbb{R}^{n \times l}$, and $b \in \mathbb{R}^n$. With a slight abuse of notation, the lower-level objective function value $f(x,y)$ is now given by $f^\top y$. If the lower-level objective function linearly depends on the upper-level decision x, the corresponding term is constant at the lower level and does not influence the minimization. It is therefore omitted in (2.6). On the other hand, the lower-level constraint function $g(x,y)$ is now given by $Cx + Dy - b$, which also contains all linear constraints defining Y.

For a fixed upper-level decision $x \in \Omega_x$ and lower-level dual variables $\lambda \in \mathbb{R}^n_{\geq 0}$, the lower-level dual problem reads

$$\max_{\lambda \geq 0} \quad \lambda^\top (b - Cx) \quad \text{s.t.} \quad D^\top \lambda = f.$$

The dual feasible region is independent of the upper-level variables and is denoted by

$$\Omega_{\mathrm{D}} := \left\{ \lambda \in \mathbb{R}^n_{\geq 0} \colon D^\top \lambda = f \right\}.$$

Since the lower level (2.6) is an LP, weak duality is always satisfied, i.e., for a lower-level primal-dual feasible point (y, λ),

$$f^\top y \geq \lambda^\top (b - Cx)$$

always holds. Lower-level optimality of y can thus be ensured by imposing that a lower-level dual feasible λ exists such that strong duality holds for the pair (y, λ). The resulting *strong-duality reformulation* of Problem (2.1) is obtained by

$$\max_{x,y,\lambda} \quad F(x, y) \quad \text{s.t.} \quad (x, y) \in \Omega, \ \lambda \in \Omega_{\mathrm{D}}, \ f^\top y \leq \lambda^\top (b - Cx). \tag{2.7}$$

Bilevel feasibility can also be achieved by imposing the Karush–Kuhn–Tucker (KKT) conditions for the lower level; see, e.g., the book by Boyd and Vandenberghe (2004). In the linear case, they are necessary and sufficient conditions for the optimality of the lower level and characterize the follower's rational reaction. The KKT stationarity conditions are equivalent to the lower-level dual feasibility $\lambda \in \Omega_{\mathrm{D}}$. The *KKT reformulation* of Problem (2.1) is obtained by replacing the strong-duality constraint in (2.7) by the KKT complementarity conditions, yielding

$$\max_{x,y,\lambda} \ F(x, y) \ \text{s.t.} \ (x, y) \in \Omega, \ \lambda \in \Omega_{\mathrm{D}}, \ \lambda_i (Cx + Dy - b)_i \leq 0, \ i \in \{1, \dots, n\}. \tag{2.8}$$

Observe that both the strong-duality and the KKT reformulations are often applicable to more general bilevel problems if $f(x, \cdot)$ is convex and $g(x, \cdot)$ is concave for a given $x \in \Omega_x$, and Y is a convex set. In particular, if the lower level satisfies some constraint qualification, which in the convex case usually is Slater's condition, then linear duality theory can easily be extended; see, e.g., the book by Boyd and Vandenberghe (2004). In this case, strong duality of the lower level still holds and the KKT conditions are still necessary and sufficient for lower-level optimality.

In the next section, we review some of the challenges that arise in solving bilevel problems and some methods found in the literature to tackle the single-level reformulations.

2.3 Challenges and Solution Approaches

In the literature, a variety of solution approaches exist to solve the three single-level reformulations of Section 2.2, but bilevel optimization is by no means easy. If in addition to a linear lower level (2.6), the functions F and G are linear and the set X is a polyhedron, then Problem (2.1) is a *linear bilevel problem* or more explicitly an *LP-LP bilevel problem*. For this problem class, the upper and the lower level are LPs and it is thus the easiest instantiation of bilevel optimization. Nonetheless, LP-LP bilevel optimization has been shown to be NP-hard by Jeroslow (1985). Later, Hansen et al. (1992) even prove it is strongly NP-hard by reduction from KERNEL. Audet et al. (1997) establish the link between LP-LP bilevel problems and mixed-integer linear problems (MILP). The authors observe that the bilevel-feasible points of

$$y = 0, \; y \in \arg\max_{\bar{y}} \{\bar{y} \colon \bar{y} \leq x, \; \bar{y} \leq 1 - x\}$$

are exactly given by $x \in \{0, 1\}$ and $y = 0$. This example shows, in particular, that MILPs are a special case of LP-LP bilevel problems and illustrates the inherent nonconvex nature of bilevel optimization. It is well known that if an LP-LP bilevel problem is feasible, an optimal solution occurs at a vertex of the shared constraint set Ω; see Bard (1998). These problems can therefore be solved by vertex enumeration. One example is the K^{th} best algorithm of Bialas and Karwan (1984). The algorithm starts by computing an optimal vertex of the high-point relaxation (2.4) and then iteratively generates adjacent vertices of Ω until a bilevel-feasible vertex is found. The first bilevel-feasible vertex found in this process is then the bilevel-optimal solution.

One of the major challenges when using the optimal-value-function reformulation (2.5) is that the optimal value function φ of the lower level is not explicitly known and difficult to compute in general. In mixed-integer linear bilevel optimization, Bolusani and Ralphs (2020) discuss that φ can in some cases be approximated iteratively using a Benders-like approach. For a (continuous) linear lower level (2.6) that is bounded for all $x \in \Omega_x$, it is in theory possible to explicitly express φ over the set of vertices of Ω_{D}, denoted by $\operatorname{vert}(\Omega_{\mathrm{D}})$. For such a linear lower level, the feasible domain Ω_{D} of the lower-level dual problem is independent of the upper-level variables x and strong duality holds. The optimal value function can thus be equivalently defined by the lower-level primal or dual LPs. For any upper-level decision $x \in \Omega_x$, it is given by

$$\varphi(x) = \max_{\lambda \in \Omega_{\mathrm{D}}} \left\{ \lambda^\top (b - Cx) \right\} = \max_{\lambda \in \operatorname{vert}(\Omega_{\mathrm{D}})} \left\{ \lambda^\top (b - Cx) \right\}, \tag{2.9}$$

where the second equality follows from the fact that a solution of a bounded LP is attained at a vertex. In general, this approach requires to compute a possibly exponential number of vertices for the lower-level dual problem, which is a hard task itself. However in [FP5], we exploit the structure of a bilevel problem arising in the European gas market to give an explicit and tractable formula for φ. This is discussed in greater detail in Section 4.4.

As a consequence of (2.9), the optimal value function of an LP is a piecewise-linear and convex function. This renders Problem (2.5) a nonconvex optimization problem, even if all other functions are linear and all variables are continuous. The same observation holds for the strong-duality reformulation (2.7) and the KKT reformulation (2.8). The strong-duality constraint introduces bilinear terms of upper-level variables x and lower-level dual variables λ. If the linking variables are bounded integers and if appropriate bounds on the lower-level dual variables can be determined, these bilinear terms can be linearized. Zare et al. (2019) show that the resulting reformulation can outperform a KKT-based approach for bilevel problems with a large number of lower-level constraints. Bilinear products of continuous variables can also be tackled combining classic convex envelopes and spatial branching and are nowadays solvable by generic mixed-integer solvers such as CPLEX (Klotz 2017) or Gurobi (Achterberg 2019). While the strong-duality constraint captures aggregated information of all KKT complementarity conditions, the KKT reformulation (2.8) is a special case of mathematical programs with complementarity constraints (MPCC), or more generally, of mathematical programs with equilibrium constraints (MPEC). The techniques specific to MPCC and MPEC are however outside of the scope of this dissertation, but we refer the interested reader to, e.g., Luo et al. (1996) or Outrata et al. (2013). To the best of our knowledge, the KKT reformulation was first discussed by Fortuny-Amat and McCarl (1981). Ye and Zhu (1995) show that standard constraint qualifications are violated at every feasible point of (2.8). Thus, nonlinear solvers can usually not be applied to tackle these problems.

Here, we focus on the links between bilevel problems and 0-1-optimization, and the disjunctive nature of the KKT complementarity conditions. Among the most promising solution approaches are branch-and-bound techniques based on Problem (2.8). While the idea to branch on violated complementarity conditions is already discussed by Fortuny-Amat and McCarl (1981), an actual branch-and-bound algorithm is proposed by Bard and Moore (1990). Novel branching rules specific to bilevel optimization have been studied by Hansen et al. (1992). Based on the 0-1-structure underlying bilevel optimization, Audet et al. (2007b) adapt classic MILP cutting planes and present a branch-and-cut algorithm for the linear bilevel problem. On the other hand, disjunctive cuts based on violated complementarity conditions have been developed in Audet et al. (2007a).

Fortuny-Amat and McCarl (1981) already observed that complementarity constraints can be modeled using special ordered sets of type 1 (SOS1); see Beale and Tomlin (1970). Modern mixed-integer solvers commonly support SOS1 and thus allow to solve bilevel problems without a need to re-implement a branch-and-bound framework; see Pineda et al. (2018) and Kleinert and Schmidt (2020a), as well as Section 2.5. However, the most common approach in the literature on LP-LP bilevel problems, and the technique employed by Fortuny-Amat and McCarl (1981), is to use a big-M linearization of the KKT complementarity conditions to transform (2.8) into a mixed-integer optimization problem. Therefore, every complementarity constraint $\lambda_i(Cx+Dy-b)_i \leq 0$, $i \in \{1,\dots,n\}$, is replaced with a new binary variable $z_i \in \{0,1\}$ together with the constraints

$$\lambda_i \leq M_{\mathrm{D}} z_i, \quad (Cx + Dy - b)_i \leq M_{\mathrm{P}}(1 - z_i), \tag{2.10}$$

where $M_{\mathrm{P}}, M_{\mathrm{D}} \geq 0$ are sufficiently large big-M constants. The benefits of this approach have, among others, been studied for LP-LP bilevel problems for which the resulting reformulation becomes an MILP. It allows to solve the problem with solvers such as CPLEX and Gurobi and thereby exploiting a collection of MILP-tailored heuristics and cutting planes out-of-the-box. An important step in this transformation is the choice of M_{P} and M_{D}, which can significantly influence the performance and correctness of the reformulation.

2.4 Bilevel-Correct Big-Ms

When applying the linearization (2.10) to solve the KKT reformulation of a bilevel problem, the choice of M_{P} and M_{D} is crucial. Larger values lead to weaker relaxations when omitting the integrality of the variables z, which results in a decrease in performance of branch-and-bound methods. On the contrary, if the big-Ms are chosen too small, the solution of Problem (2.8) with linearized KKT complementarity constraints (2.10) might not be optimal for the original bilevel problem. Pineda and Morales (2019) have shown that a commonly used heuristic for computing big-Ms can lead to suboptimal bilevel solutions. This leads us to define correct big-Ms for bilevel optimization.

Definition 2.1. Constants $M_{\text{P}}, M_{\text{D}} \geq 0$ are *bilevel-correct* big-Ms if the bilevel problem (2.1) with linear lower level (2.6) and the KKT reformulation (2.8) with linearized complementarity constraints (2.10) admit the same optimal value.

Intuitively, big-Ms need to be chosen large enough not to cut off all bilevel-optimal solutions. In [FP1], we discuss two sufficient conditions for bilevel-correctness of big-Ms in LP-LP bilevel optimization. We briefly present the results in the following and discuss their implications. We focus on the selection of $M := M_{\text{D}}$. In practice, primal variable bounds are often given or can be deduced from the data of the problem. Here, we assume that the shared constraint set Ω is nonempty and bounded. Thus, M_{P} can easily be derived. Additionally, we will observe that the selection of M_{D} is already a hard task, and therefore the same holds true for the selection of both big-Ms.

If a bilevel problem is feasible, the lower-level primal and dual problems have a finite optimal value. Consequently, in an LP-LP bilevel problem, for every upper-level decision $x \in \Omega_x$, there is a pair of lower-level primal and dual vertices (y, λ) optimal for their respective LPs. In Section 3 of [FP1], we consider the choice of M such that no vertex of the lower-level dual feasible region is cut off in the KKT reformulation (2.8) with linearized complementarity constraints (2.10). It then follows that all bilevel-feasible points are also preserved and thus that M is bilevel-correct. We need to choose $M \geq 0$ such that $\lambda_i \leq M$ holds for all vertices $\lambda \in \operatorname{vert}(\Omega_{\text{D}})$ and for all $i \in \{1, \dots, n\}$. In other words, the choice of M preserves all vertices of the lower-level dual problem if and only if

$$M \geq \max\left\{\lambda_i \colon \lambda \in \operatorname{vert}(\Omega_{\text{D}})\right\}, \quad i \in \{1, \dots, n\}. \tag{2.11}$$

Since we assume the boundedness of Ω, it particularly implies that the lower-level primal feasible region is bounded for every upper-level decision $x \in \Omega_x$. A result by

Clark (1961), more generally stated in Theorem 1 and its corresponding corollary by Williams (1970), claims that the dual feasible region Ω_{D} is then necessarily unbounded. Validating M w.r.t. (2.11) therefore requires finding optimal vertices maximizing linear objective functions over the unbounded polyhedron Ω_{D}. Theorem 4.1 of Fukuda et al. (1997) implies that the latter task is strongly NP-hard. Since we want to guarantee M is a valid upper bound on the vertices of the lower-level dual problem, we directly derive the following result.

Theorem 2.2 (Theorem 2 in [FP1])**.** *For a given $i \in \{1, \dots, n\}$ and $M \in \mathbb{Q}_{\geq 0}$, deciding if $\lambda_i \leq M$ holds for all $\lambda \in \operatorname{vert}(\Omega_D)$ is strongly coNP-complete.*

As a consequence, there is no polynomial-time algorithm to validate a given M w.r.t. (2.11) unless P = NP. Similarly, the tightest big-M preserving all vertices of Ω_{D}, given by

$$M = \max_{i \in \{1,\dots,n\}} \max_{\lambda \in \operatorname{vert}(\Omega_{\text{D}})} \lambda_i,$$

cannot be computed efficiently in that case.

If we require that all vertices are preserved in the lower-level dual problem, the choice of M could however be very conservative. In general, it is enough to preserve bilevel-feasible points and therefore it is sufficient to preserve only those vertices optimal for some upper-level decision $x \in \Omega_x$. This proxy to validate bilevel-correct big-Ms is discussed in Section 4 of [FP1]. We derive the main result of this section in a slightly adapted way, which the author of this dissertation believes to be more straightforward, but is equivalent to what is presented in our article. First, we make the following simplifying assumption on the uniqueness of lower-level solutions.

Assumption 2.3. For every upper-level decision $x \in \Omega_x$, the lower level admits a unique pair $(y^*(x), \lambda^*(x))$ of primal and dual optimal solutions.

This assumption can be very restrictive. If the lower-level primal solution is not uniquely determined, analyzing the structure of bilevel-feasible points is even more difficult; see Chapter 7 of Dempe (2002). The uniqueness of the lower-level dual solution can be guaranteed by additionally requiring that the lower level satisfies the linear independence constraint qualification (LICQ) at the unique lower-level primal solution $y^*(x)$ for every upper-level decision $x \in \Omega_x$; see Chapter 12 of Nocedal and Wright (2006). Despite this extreme simplification, we show that preserving bilevel-feasible points is a hard task. As a consequence, the problem must be at least as hard without Assumption 2.3.

For a given upper-level decision $x \in \Omega_x$, the unique solution $\lambda^*(x)$ of the lower-level dual problem is obtained by solving an LP. It can thus be efficiently checked that the corresponding bilevel-feasible point $(x, y^*(x))$ is not cut off, i.e., if

$$M \geq \lambda_i^*(x), \quad i \in \{1, \dots, n\}, \tag{2.12}$$

holds. To preserve all bilevel-feasible points, (2.12) must be satisfied for every upper-level decision $x \in \Omega_x$. As a consequence, we obtain the following result for which we exceptionally also present a proof. The proof in this dissertation is more direct than the one presented in [FP1] and might thus be easier to follow.

Theorem 2.4 (Theorem 3 in [FP1]). *Suppose that Assumption 2.3 holds, then $M \geq 0$ is bilevel-correct if*

$$M \geq \max_{x,y,\lambda} \left\{ \lambda_i \colon (x,y) \in \Omega,\, \lambda \in \Omega_D,\, \lambda_{i'}(Cx + Dy - b)_{i'} \leq 0,\, i' \in \{1, \dots, n\} \right\} \quad (2.13)$$

holds for every $i \in \{1, \dots, n\}$.

Proof. By definition, $x \in \Omega_x$ holds if and only if there exists a lower-level primal decision y such that $(x, y) \in \Omega$. Therefore, $M \geq 0$ is bilevel-correct, if

$$M \geq \max_{(x,y) \in \Omega} \lambda_i^*(x), \quad i \in \{1, \dots, n\}.$$

Since the lower level is an LP for a given x, we can define $\lambda^*(x)$ by means of the KKT optimality conditions of the lower-level problem (2.6); see Section 2.2. □

Validating the bilevel-correctness of M w.r.t. Theorem 2.4 requires optimizing different objective functions over the feasible set of the KKT reformulation (2.8). The tightest M w.r.t. Theorem 2.4 is obtained by setting equality in (2.13). Computing such a big-M is therefore as hard as solving the initial bilevel problem.

Both proxies for bilevel-correctness discussed in [FP1] abstract from the optimality of the upper level. Even when focusing only on preserving bilevel-feasible points, the task of selecting correct big-Ms for general bilevel problems with a linear lower level is very challenging. Considering bilevel-optimal solutions would add an additional layer of complexity. When using the KKT reformulation (2.8) with linearized complementarity constraints (2.10), provably correct M_P and M_D can still be derived from problem-specific knowledge. In [FP5], we exploit the structure of a problem in the European gas market to derive bilevel-correct big-Ms. Since the physics of gas are well-understood in our models, it is possible to determine ranges within which exists at least one bilevel-optimal solution. This allows us to make use of the KKT reformulation with linearized complementarity constraints as a benchmark in our computational study. In our work, it also becomes apparent that in order to be provably correct, the choice of big-Ms might be very conservative and thus lead to slow performance. However, we do not observe any slowdowns resulting from our choice of big-Ms and therefore refrain from further improvement attempts.

Alternatively, big-M-free approaches can be applied to Problem (2.8) directly. In the case of LP-LP bilevel optimization, this can be done, e.g., using the previously mentioned K^{th} best algorithm by Bialas and Karwan (1984). Furthermore, MILP-tailored techniques are often applied in the literature; see the recent survey article Kleinert et al. (2021a). In the next section, we discuss valid inequalities to be used in a big-M-free branch-and-cut framework, in which we directly branch on violated complementarity constraints.

2.5 Valid Inequalities for a Big-M-Free Branch-and-Cut

In Section 2.3, we have discussed the possibility to branch on the complementarity constraints of the KKT reformulation (2.8), as proposed, e.g., by Bard and

Moore (1990). In that way, a large class of bilevel problems can be tackled using state-of-the-art branch-and-bound or branch-and-cut algorithms without relying on the big-M linearization (2.10). The results of Section 2.4 have proven that the big-M linearization of the KKT reformulation must be applied with great care.

Compared to the vast literature on MILP-specific branch-and-cut techniques, there has only been a small stream of research into LP-LP bilevel-tailored branching algorithms. In [FP2], we study a branch-and-cut framework for LP-LP bilevel optimization as a big-M-free alternative to the linearized KKT approach. We follow the notations of [FP2] and therefore consider an LP-LP bilevel problem in its optimistic form given by

$$\min_{x,y} \quad c^\top x + d^\top y \quad \text{s.t.} \quad Ax + By \geq a, \ y \in \mathcal{S}(x), \tag{2.14}$$

where $\mathcal{S}(x)$ denotes the set of optimal solutions of

$$\max_{y} \quad f^\top y \quad \text{s.t.} \quad Dy \leq b - Cx$$

and $c \in \mathbb{R}^k$, $d, f \in \mathbb{R}^l$, $A \in \mathbb{R}^{m\times k}$, $B \in \mathbb{R}^{m\times l}$, $a \in \mathbb{R}^m$, $C \in \mathbb{R}^{n\times k}$, $D \in \mathbb{R}^{n\times l}$, and $b \in \mathbb{R}^n$. In that case, the shared constraint set is defined by

$$\Omega = \{(x, y) \colon Ax + By \geq a, \ Cx + Dy \leq b\},$$

which we assume to be nonempty and bounded. The KKT reformulation then reads

$$\begin{aligned} \min_{x,y} \quad & c^\top x + d^\top y && (2.15a)\\ \text{s.t.} \quad & (x, y) \in \Omega, \ \lambda \in \Omega_{\mathrm{D}}, && (2.15b)\\ & \lambda_i (b - Cx - Dy)_i \leq 0, \quad i \in \{1, \dots, n\}. && (2.15c) \end{aligned}$$

Branching on violated complementarity constraints can be summarized as follows. First, the high-point relaxation of Problem (2.15), i.e., the problem without Constraints (2.15c), is solved at the root of the branch-and-bound tree. If Constraints (2.15c) are satisfied, the root solution is also optimal for (2.15). Otherwise, there exists $i \in \{1, \dots, n\}$ such that complementarity constraint i is violated, i.e., $\lambda_i(b - Cx - Dy)_i > 0$ holds. Two new nodes are created adding the constraint $\lambda_i = 0$ or $(b - Cx - Dy)_i = 0$, respectively. Thus, bilevel-feasibility is ensured by iteratively adding KKT complementarity conditions back into the problem. The presented complementarity-based branching can be implemented in most modern solvers using SOS1; see also Pineda et al. (2018) and Kleinert and Schmidt (2020a). A slack variable $s_i := (b - Cx - Dy)_i$ is introduced for every $i \in \{1, \dots, n\}$, then Constraints (2.15c) can equivalently be written as

$$s_i = (b - Cx - Dy)_i, \quad \{s_i, \lambda_i\} \text{ SOS1}, \quad i \in \{1, \dots, n\}.$$

In this form, the problem could directly be solved by a state-of-the-art solver handling SOS1, like CPLEX or Gurobi.

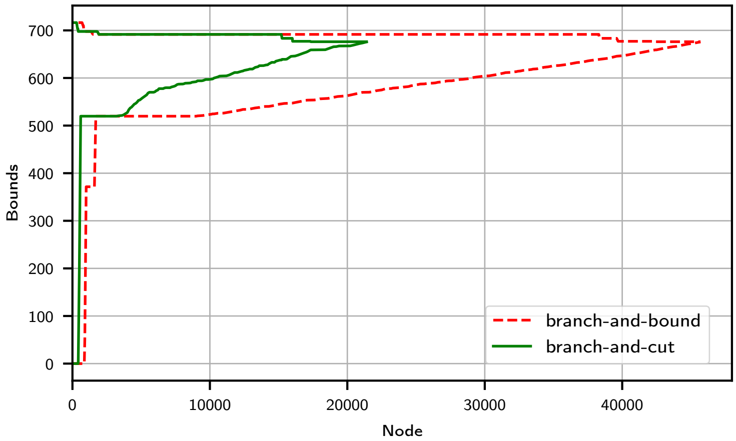

Figure 2.1: Evolution of lower and upper bounds over the course of visited nodes in a complementarity-based branching for an LP-LP bilevel problem (taken from [FP2]).

Although being a big-M-free approach, there is a notable drawback. At the root, i.e., in the high-point relaxation, lower-level primal variables y and dual variables λ are completely decoupled, since the complementarity constraints (2.15c) have been omitted. This leads to a weak relaxation, which in turn can lead to slow convergence. The dashed line in Figure 2.1 shows the evolution of upper and lower bounds during a branch-and-bound run on an LP-LP knapsack interdiction instance. An almost optimal solution is quickly found, but many nodes need to be visited to close the gap. Some valid inequalities for general LP-LP bilevel problems have been discussed by Audet et al. (2007a,b) and Wu et al. (1998) that can be used to extend the complementarity-based branching to a branch-and-cut algorithm. However, some of these valid inequalities require additional binary variables in their modeling or might fail to introduce a coupling of the lower-level primal and dual variables. In an effort to introduce this coupling, we develop a family of new primal-dual valid inequalities in [FP2], based on the lower-level strong-duality constraint. The solid line in Figure 2.1 shows the effect of a branch-and-cut approach based on these valid inequalities for the same instance as before. The number of nodes visited during the branching is cut in half and optimality of the initially found solution can be proven much faster. We briefly discuss the derivation of the linear valid inequalities in the following. For more detail, we refer to Section 3 of [FP2].

The strong-duality constraint $\lambda^\top b - \lambda^\top Cx - f^\top y \leq 0$ of the lower level is obtained by aggregating the KKT complementarity conditions (2.15c) for all $i \in \{1, \dots, n\}$ and using lower-level dual feasibility $\lambda \in \Omega_{\mathrm{D}}$ to substitute $D^\top \lambda$ by f. All variables in the LP-LP bilevel problem (2.14) are continuous. Consequently, the term $\lambda^\top Cx$ is bilinear and cannot be linearized easily, as opposed to problems with integer variables; see Zare et al. (2019). Strong duality can still be exploited to derive a valid inequality. A very simple idea is to replace the nonconvex term by considering an upper bound C_i^+ on $C_{i\cdot}x$, where $C_{i\cdot}$ denotes the ith row of C. Since we assume that the shared constraint set Ω is bounded, finite bounds $C^+ = (C_i^+)_{i=1,\dots,n}$ can be derived by variable bounds on x and the resulting inequality

$$\lambda^\top b - \lambda^\top C^+ - f^\top y \leq 0 \tag{2.16}$$

is obviously valid. Generating this valid inequality is computationally inexpensive, but it can be arbitrarily bad depending on the quality of the variable bounds on x. Stronger bounds can be computed by solving auxiliary LPs

$$C_i^+ := \max_{x,y,\lambda} \{C_{i\cdot}x \colon (x, y, \lambda) \in (\Omega \times \Omega_{\mathrm{D}}) \cap \mathcal{C}\}, \quad i \in \{1, \dots, n\},$$

where $\mathcal{C}$ is a constraint set containing previously generated valid inequalities (2.16) as well as branching conditions at the current branch-and-bound node. These tighter bounds are locally valid for nodes in the subtree rooted at the current branch-and-bound node. In that way, locally valid inequalities can be generated at every node.

Good bounds could already be readily available in modern solvers that regularly apply some form of bound tightening; see, e.g., Belotti et al. (2010). The valid inequalities (2.16) can then be generated at any branch-and-bound node using that information. To the best of our knowledge, this information is however not accessible to the users of CPLEX or Gurobi. In [FP2], we have therefore implemented a complementarity-based branching using CPLEX callbacks and set up our own bookkeeping of the set $\mathcal{C}$. Different branching rules for LP-LP bilevel problems are discussed in the literature, e.g., by Hansen et al. (1992). For simplicity, we have decided to branch on the most violated complementarity constraint. Various parameterizations of the branch-and-cut algorithm are studied, for which cuts are separated locally at different depths of the branch-and-bound tree. The computational study has shown that adding a cut only at the root node, i.e., a cut-and-branch algorithm, results in the best trade-off between the costs of cut separation and the overall solution time. In this dissertation, we only illustrate the effect of adding (2.16) at the root node and refer the reader to Section 4 of [FP2] for a more detailed insight into the instances used in the computational study and the full analysis.

Our computational analysis is based on a test set of 1017 LP-LP instances derived from the literature; see Kleinert and Schmidt (2020b) and [FP2]. Among these instances we retain 919 that could be solved by either the branch-and-bound or the cut-and-branch approach within a time limit of one hour. To eliminate instances that are too easy, we only consider those for which one method has a running time of at least 10 s. The impact of the valid inequality on the remaining 374 instances is illustrated in log-scaled performance profiles according to Dolan and Moré (2002). For every instance i in our test set and every solution approach s, we compute the ratio $r_{i,s} := p_{i,s} / \min\{p_{i,s} \colon s \in S\}$, where $S = \{\text{branch-and-bound}, \text{cut-and-branch}\}$ is the set of considered methods and $p_{i,s}$ is the performance of s on i w.r.t. a given measure. For every method s and $\tau \geq 1$ (log-scaled x-axis), the performance profile then shows the fraction of instances (y-axis) that admit a ratio $r_{i,s} \leq \tau$, i.e., s solves i with a performance that is within a factor τ of the best approach. Figure 2.2 shows log-scaled performance profiles w.r.t. the number of branch-and-bound nodes (left)

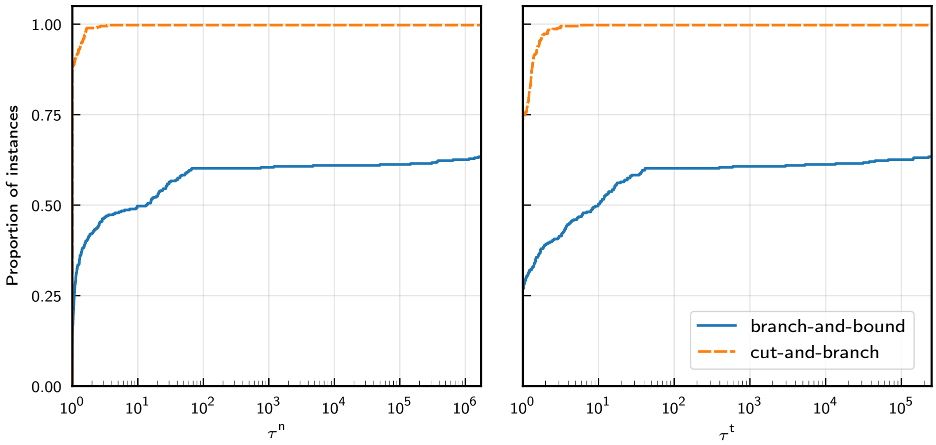

Figure 2.2: Log-scaled performance profile of branch-and-bound node counts (left) and running times (right) (adapted from [FP2]).

and the running time in seconds (right). Our implemented branching on worst-violated complementarity constraints solves 237 instances. In contrast, all except one, i.e., 373, are solved by the cut-and-branch algorithm equipped with our valid inequality at the root node. Significantly fewer nodes need to be considered during the branching if a valid inequality is added at the root node. The resulting running times are also shorter and already account for the time necessary for the cut separation. This figure thus suggests that Inequalities (2.16) have the potential to speed up the resolution of LP-LP bilevel problems in complementarity-based and big-M-free branch-and-cut frameworks. It is likely that this effect can be traced back to the reintroduction of a coupling of lower-level primal and dual variables in the root node relaxation. If variable bound information present in state-of-the-art solvers is exploited, Inequalities (2.16) can be generated with very little overhead. They can then be integrated in a full branch-and-cut framework and added locally at various nodes in the branch-and-bound tree to obtain faster convergence as discussed for Figure 2.1.

3

Gas Transport and Market System

Besides bilevel optimization, the other main topic of this dissertation is concerned with the feasibility of special capacity-right contracts in the European entry-exit gas market. In this chapter, we introduce the modeling of stationary gas flows used throughout this work as well as the organization of the European gas market. In Section 3.1, we begin with a brief overview of the physics underlying gas transport. Section 3.2 is then devoted to the introduction of a potential-based flow model used to approximate the physics of gas. In Section 3.3, we discuss the organization of the European entry-exit gas market. Therein, we particularly focus on the two types of capacity-right contracts at the core of this market structure, namely bookings and nominations. Finally, we review some results from the literature related to our work in Section 3.4.

3.1 Foundations of Gas Transport

We begin our presentation by an introduction to the foundations of gas transport and the network elements considered in this dissertation. We mostly follow Chapter 2 by Fügenschuh et al. (2015) of the book edited by Koch et al. (2015). Gas is injected into or withdrawn from the network at *entries* or *exits*, respectively. Entries represent supply locations, like natural gas fields, but also interconnection points to other networks. Similarly, exits might also be interconnection points and, more commonly, represent various customers. The majority of elements in a network are *pipes*, in which gas might be subject to a drop in pressure due to friction. To additionally control the pressure levels, there are *active elements* in the network, like *compressors* that allow to increase the pressure or *control valves* that allow to decrease it. The TSO is in charge of guaranteeing the flow of gas between entry and exit points and control the active elements to ensure an operation within the technical restrictions of the network. There is a range of other network elements, that are not discussed in this dissertation. We refer to Fügenschuh et al. (2015) for a more complete overview.

The flow of gas in a pipe is governed by a system of hyperbolic nonlinear partial differential equations, called *Euler equations*; see, e.g., Feistauer et al. (2003) or Lurie (2008). Together with an adequately chosen equation of state, they allow to describe the dynamics of gas in a pipe. In this dissertation, we study stationary and isothermal gas flows, i.e., independent of time and admitting the same temperature at all points of the network. Additionally, we assume that the ram pressure term can be neglected and that the compressibility factor can be approximated by a suitable constant z_{m} along the entire pipe. Under these assumptions, the dynamics of gas flow in a pipe with constant slope s can be approximated by a well-known relation by Weymouth (1912) between inlet pressure p_{in}, outlet pressure p_{out}, and the constant mass flow q in the pipe,

$$p_{\mathrm{out}}^2 = \left(p_{\mathrm{in}}^2 - \Lambda\,|q|\,q\frac{e^S-1}{S}\right)e^{-S} \tag{3.1}$$

with

$$\Lambda := \lambda\frac{R_{\mathrm{s}}z_{\mathrm{m}}TL}{A^2D}, \quad S := \frac{2gsL}{R_{\mathrm{s}}z_{\mathrm{m}}T}.$$

It quantifies the pressure loss caused by flow in a pipe. R_{s} is the specific gas constant and T the constant gas temperature across the network. The pressure loss also depends on pipe-specific characteristics such as its diameter D, its cross-sectional area A, its length L, and its slope s. Especially, for inclined pipes there is an additional gravitational influence on the gas flow, justifying the presence of the gravitational acceleration constant g in (3.1). Note that (3.1) is not defined for horizontal pipes, i.e., $s = 0$ and therefore $S = 0$. Taking the limit for $S \to 0$ of the right-hand side of (3.1), we obtain the corresponding relation for horizontal pipes

$$p_{\mathrm{out}}^2 = p_{\mathrm{in}}^2 - \Lambda|q|q. \tag{3.2}$$

The influence of friction at the inner walls of the pipe is summarized in the friction factor λ. We use the approximation by Nikuradse (1955) given by

$$\lambda = \left(2\log_{10}\left(\frac{D}{k}\right) + 1.138\right)^{-2},$$

where k is the roughness of the pipe that quantifies the deviation of its inner walls from a perfectly smooth shape. Finally, z_{m} represents a mean value approximate of the compressibility factor; see Saleh (2002).

The dynamics of gas in active elements, especially compressors, are usually more involved, see Odom and Muster (2009), and are out of the scope of this dissertation. The problems discussed herein are already very challenging on networks without controllable elements, called *passive networks* in the remainder of this dissertation. If *active networks* are considered, we thus use strongly simplified models for the active elements, which we present in the next section.

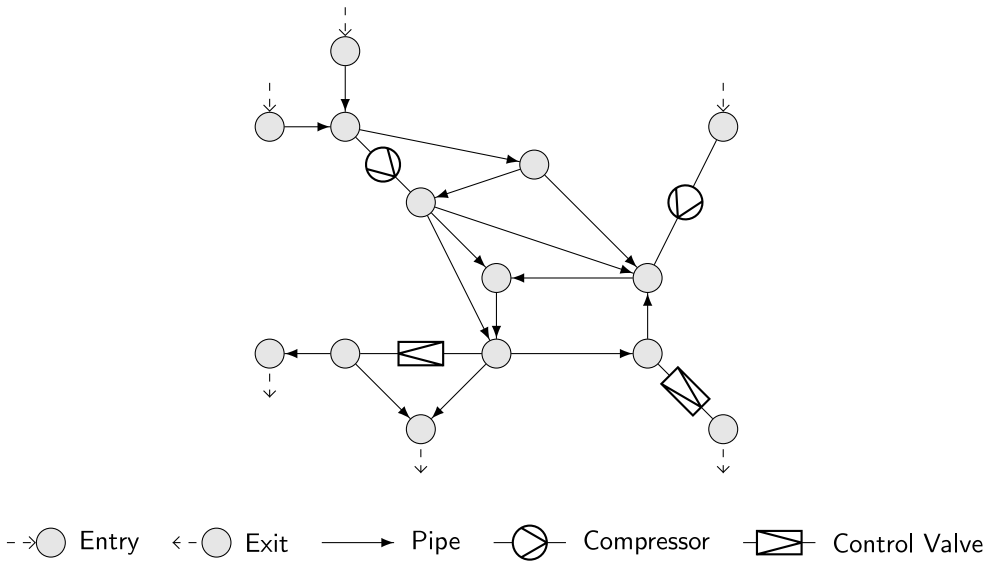

Figure 3.1: Stylized example of a gas network with active elements (adapted from [FP5]).

3.2 A Potential-Based Flow Model for Gas Transport

In [FP3; FP4; FP5], we model stationary gas flows by a *potential-based flow model*. The gas network is represented by a directed and weakly connected graph $G = (V, A)$, i.e., the corresponding undirected graph is connected. The set of nodes V 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 A is partitioned into pipes A_{pipe} and active elements A_{act}, which are further split into compressors A_{cm} and control valves A_{cv}. Figure 3.1 shows a stylized example of a network with active elements. Entry and exit nodes are symbolized by dashed arcs entering and leaving the nodes, respectively. Pipes are represented by solid arcs between two nodes, whereas compressors and control valves are indicated by their respective technical symbols. To present the potential-based flow model, we first introduce the load flow of the network G.

Definition 3.1. 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 ℓ represents the actual quantity of gas to be transported through the network. More precisely, ℓ_u is the amount of gas injected at an entry $u \in V_+$ or withdrawn at an exit $u \in V_-$.

The potential-based flow model is an extension of classic linear flows. One of the earliest studies, to the best of our knowledge, dates back to Birkhoff and Diaz (1956). In the book by Rockafellar (1984), potential-based flows are a central topic. Today, they are widely used in the literature on gas transport; see, e.g., the PhD theses by Stangl (2014), Willert (2014), Hayn (2017), and Aßmann (2019), the book edited by

Koch et al. (2015), and the survey article by Ríos-Mercado and Borraz-Sánchez (2015) as well as the references therein. The variables of the model are the flows $q = (q_a)_{a\in A}$, the potentials $\pi = (\pi_u)_{u\in V}$, and the controls of the active elements $\Delta = (\Delta_a)_{a\in A_{\text{act}}}$. For an arc $a = (u, v)$, we interpret $q_a > 0$ as flow in the direction of the arc, i.e., from u to v, and $q_a < 0$ as flow in the opposite direction. In contrast to linear flows and in addition to the flow conservation w.r.t. the load flow ℓ at every node, flows are governed by potentials. More precisely, the flow along every pipe is linked to the incident potentials. For a pipe $a = (u, v) \in A_{\text{pipe}}$, it holds that

$$\pi_u - \pi_v = \Lambda_a |q_a| q_a, \tag{3.3}$$

where $\Lambda_a > 0$ is a pipe-specific constant. For gas transport in horizontal pipes, the relations (3.2) can be rewritten as (3.3) by defining $\pi_u := p_u^2$ for every $u \in V$. In this case, potentials are thus given by the squared pressures at nodes. Groß et al. (2019) show that (3.3) can also model non-horizontal pipes. Additionally, the authors discuss that potential-based flows may be used to study DC power flow or water transport by varying the right-hand side of (3.3). Many results discussed in this thesis also apply if the right-hand side is a general potential function $f(q_a)$, as studied in [FP3]. In this case, it is assumed that f is continuous, strictly increasing, and odd.

On the other hand, active elements also influence the potentials incident to their corresponding arcs. There exist a variety of models for active elements, ranging from simple linear to sophisticated mixed-integer linear ones; see, e.g., Wu et al. (2000), Martin et al. (2006), Fügenschuh et al. (2015), and Rose et al. (2016). In this dissertation, we only consider active elements that linearly increase (compressors) or decrease (control valves) the potentials. Such linearly modeled active elements are also studied by Aßmann et al. (2019) and in the PhD thesis by Aßmann (2019). Active elements often require a certain amount of flow to function and are in bypass mode otherwise. Given an upper bound $\Delta_a^+ \geq 0$ on its operation and a minimum quantity of flow $m_a \geq 0$, an active element $a = (u, v) \in A_{\text{act}}$ can linearly modify potentials by $\Delta_a \in [0, \Delta_a^+]$ if a sufficient amount of flow traverses a in the "correct" direction, i.e., if $q_a > m_a$ holds. We thus linearly 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 $\chi_a(q)$ is an indicator function given by

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

We can now formally define the potential-based flow model studied in this dissertation for gas transport in networks with linearly modeled active elements.

Definition 3.2. Given a load flow $\ell \in L$ on the network G, a *potential-based flow* (q, π, Δ) satisfies the following constraints

$$\sum_{a \in \delta^{\text{out}}(u)} q_a - \sum_{a \in \delta^{\text{in}}(u)} q_a = \begin{cases} \ell_u, & u \in V_+, \\ -\ell_u, & u \in V_-, \\ 0, & u \in V_0, \end{cases} \tag{3.4a}$$

$$\pi_u - \pi_v = \Lambda_a |q_a| q_a, \quad a = (u, v) \in A_{\text{pipe}}, \tag{3.4b}$$

$$\pi_u - \pi_v = \begin{cases} -\Delta_a, & a = (u, v) \in A_{\text{cm}}, \\ \Delta_a, & a = (u, v) \in A_{\text{cv}}, \end{cases} \tag{3.4c}$$

$$\Delta_a \in [0, \Delta_a^+ \chi_a(q)], \quad a \in A_{\text{act}}, \tag{3.4d}$$

$$\pi_u \in [\pi_u^-, \pi_u^+], \quad u \in V, \tag{3.4e}$$

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 constant 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 an active element for all $a \in A_{\text{act}}$.

Constraints (3.4a) ensure flow conservation at every node of the network w.r.t. the load flow ℓ. For pipes, Constraints (3.4b) link arc flows to the incident node potentials, as previously discussed. For active elements, Constraints (3.4c) determine the change in incident node potentials according to the control. Additionally, Constraints (3.4d) guarantee that a compressor or a control valve operates in its allowed range, if the flow exceeds the minimum threshold, and is in bypass mode otherwise. Finally, due to technical restrictions of the network, potentials need to satisfy the bounds in (3.4e). Note that in [FP3], we additionally consider lower and upper bounds on the flows q. They are, however, not considered in the remaining publications [FP4; FP5] and are thus omitted in the presentation of this dissertation.

In passive networks, i.e., $A_{\text{act}} = \emptyset$, a key property of potential-based flows often exploited in this dissertation is that if feasible flows q corresponding to a given load flow ℓ exist, then they are unique. As a direct consequence of (3.4b), potential differences $\pi_u - \pi_v$ are also uniquely determined by ℓ for every $(u, v) \in A_{\text{pipe}}$. These observations lead to the following result.

Proposition 3.3 (Maugis 1977; Collins et al. 1978)**.** *Let $G = (V, A)$ be a weakly connected and passive network. If $\ell \in L$ is a balanced load flow, i.e., ℓ satisfies $\sum_{u \in V_+} \ell_u = \sum_{u \in V_-} \ell_u$, then every feasible point (q, π) of (3.4a) and (3.4b) admits the same unique flows $q(\ell)$. Furthermore, for two feasible points $(q(\ell), \pi)$ and $(q(\ell), \tilde{\pi})$, there exists $\tau \in \mathbb{R}$ such that $\tilde{\pi}_u = \pi_u + \tau$ holds for every $u \in V$.*

This uniqueness holds for general passive networks and is a major difference to linear flow models, where flows along cycles can be constantly increased or decreased up to a capacity and the resulting flows remain feasible for the given load flow. Equivalently, this means that in potential-based flow networks, the split of flows across multiple paths between two given nodes in the network is uniquely determined.

Proposition 3.3 is derived in early works by Maugis (1977) and Collins et al. (1978). Therein, it is observed that (3.4a) and (3.4b) are the KKT optimality conditions of a convex min-cost flow problem with a strictly convex objective function. Later, Ríos-Mercado et al. (2002) derive Proposition 3.3 using monotone operator theory. The authors observe that for a given balanced load flow ℓ on a passive network, as soon as the potential at a reference node is fixed, the flows and potentials corresponding to ℓ are uniquely determined. Many variables are thus fixed by physics. To obtain a feasible potential-based flow w.r.t. (3.4) in the passive case, it thus remains to determine a reference potential such that no bounds are violated. Under structural assumptions on the network, Proposition 3.3 can be extended to active networks, as we will discuss in Section 4.4.

3.3 The European Entry-Exit Gas Market

As a result of the liberalization, the European gas market is organized as a so-called *entry-exit* system; see the Directive and subsequent Regulation of the European Parliament and Council of the European Union (2009a,b). The goal of this market organization is to decouple gas transport and trade. The TSO operates the network and is in charge of gas transport. On the other hand, gas traders can be suppliers or demand customers and participate in the market. They require to get the traded amounts of gas shipped through the network by the TSO from entry to exit locations. Traders therefore interact with the TSO via so-called *bookings* and *nominations*. A booking is a capacity-right contract for a maximum capacity of gas at entry and exit nodes that traders can acquire in special auctions. It is usually signed some time in advance of the actual transport and fixes an upper bound on the amount of gas to be injected at entry nodes or withdrawn at exit nodes. On a day-ahead basis and up to the booked capacity, traders then nominate the planned amount of gas to be injected or withdrawn the next day at every node of the network. Traders are obliged to nominate a balanced load flow, i.e., the total amount injected equals the total amount withdrawn. By signing a booking contract, the TSO must guarantee that every nomination up to the booked capacities can be transported within the technical restrictions of the network. Formally, we thus define nominations and bookings as follows.

Definition 3.4. A *nomination* is a balanced load flow $\ell \in L$, i.e., ℓ satisfies $\sum_{u\in V_+} \ell_u = \sum_{u\in V_-} \ell_u$. The set of nominations is denoted by N. A *booking* is a load flow $b \in L$ and a nomination ℓ is *booking-compliant* if $\ell_u \le b_u$ holds for all $u \in V$. The set of booking-compliant nominations is denoted by $N(b)$.

In this dissertation, we define the feasibility of a nomination using the potential-based flow model for stationary gas transport presented in Section 3.2.

Definition 3.5. The nomination $\ell \in N$ is *feasible* if there exists a feasible potential-based flow for ℓ, i.e., a feasible point (q, π, Δ) of (3.4).

To assess the feasibility of a nomination ℓ, it therefore suffices to determine flows q, potentials π, and controls Δ for the active elements that allow to transport ℓ within the restrictions of the network, i.e., satisfying especially the bounds (3.4d) and (3.4e). The feasibility of a booking, on the other hand, is defined by the feasibility of all infinitely many booking-compliant nominations.

Definition 3.6. The booking $b \in L$ is *feasible* if all booking-compliant nominations $\ell \in N(b)$ are feasible, i.e., the booking b is feasible if

$$\forall \ell \in N(b)\ \exists (q, \pi, \Delta) \text{ satisfying (3.4)}. \tag{3.5}$$

Consequently, to check the feasibility of a booking, all booking-compliant nominations need to admit a feasible potential-based flow. In particular, the TSO can apply different settings to the active elements for each individual nomination. In that sense, verifying the feasibility of a booking can be classified as an adjustable, respectively two-stage, robust feasibility problem; see, e.g., Ben-Tal et al. (2009) and Yanıkoğlu et al. (2019).

In addition to bookings and nominations, the entry-exit market organization encompasses various different contract types and additional rules not discussed in this dissertation. For an in-depth discussion of the market structure, we refer to Gotzes et al. (2015). Furthermore, Rövekamp (2015) discusses the historical evolution of European directives and regulations for gas transport and markets as well as their transfer to the national law on the example of Germany.

Our main focus is on the problem faced by the TSO to ensure the transportability of all nominations in compliance with booked capacities. We now shortly explain how our study of feasible bookings fits into the bigger picture of the entry-exit gas market. Grimm et al. (2019) present a four-level model for an idealized version of the European gas market. In this setting, the TSO is regulated and gas traders act under perfect competition. To decouple gas transport and trade, the TSO announces so-called *technical capacities* at entry and exit nodes at the first level. Identical to bookings studied in this dissertation, technical capacities are determined such that all possibly resulting nominations within these capacities are feasible. This allows the market participants to compete, while disregarding any aspects of the subsequent transport. At level two, traders compete for the technical capacities announced by the TSO to obtain their bookings. Level three then models the interaction at the day-ahead markets and the nomination process in compliance with these bookings. By definition of the technical capacities, the fourth level, i.e., the transport of nominations by the TSO, is guaranteed to be feasible for any decisions taken at level two and three. Technical capacities are thus constrained by the adjustable robust feasibility of the form (3.5) of all compliant nominations, which is exactly the problem of feasible bookings studied in this dissertation. In this sense, technical capacities can be interpreted as bookings. Since a TSO is encouraged to offer the largest possible technical capacities in the entry-exit gas market organization, the problem of checking the feasibility of bookings, or equivalently of technical capacities, is of central importance. The results and properties discussed in Chapter 4 play a key role to analyze the adjustable robust constraint on technical capacities in the TSO's problem at the first level; see Böttger et al. (2020) and Schewe et al. (2020a), where results of [FP3] are used to replace the adjustable robust constraint in the model by Grimm et al. (2019).

3.4 Results from the Literature

First definitions of bookings and structural insights based on small examples are given by Szabó (2012). The earliest more systematic studies concerning the feasibility of bookings in the European entry-exit gas market are found in the PhD theses by Willert (2014) and Hayn (2017). While Willert (2014) mostly discusses the validation of nominations, some first insights on technical capacities—which are particular bookings, as discussed in Section 3.3—are also given. Hayn (2017) studies the problem of checking feasible bookings, where gas physics are modeled by capacitated linear flows. In this model, there are no potentials and flows are not pressure-driven, but there are capacities on the flow on every arc. The author shows that the problem of checking feasible bookings under this setting is coNP-complete on passive networks. However, the problem is in P for tree-shaped networks. In a second step, Hayn (2017) proposes models using semi-algebraic sets, that also allow to analyze feasible bookings under potential-based flow models such as (3.4). However, only exponential upper bounds on the complexity of the corresponding decision problem are presented. Much more recently, Thürauf (2020) shows that the problem is coNP-hard on passive networks for nonlinear potential-based flows (3.4). In [FP3], we observe that the feasibility of a booking can be checked in polynomial-time on passive networks with linear potential-based flows, i.e., the right-hand sides of (3.4b) are linear functions of the flow on an arc. Furthermore, we prove that the problem is still in P for nonlinear potential-based flows, if the network is a passive tree. This result is also implied by the studies of Robinius et al. (2019). In [FP4], we show that for potential-based flows (3.4), the feasibility of a booking can still be checked in polynomial time, if the network is a single passive cycle. In Chapter 4, we will elaborate in more depth on the results of [FP3; FP4]. Figure 3.2 summarizes the complexity landscape of verifying the feasibility of bookings on passive networks. A similar figure was previously presented in [FP3] and later updated by Thürauf (2020) to include the latest insights. For active networks, Szabó (2012) shows that even verifying the feasibility of a nomination is NP-complete. On the other hand, Schewe et al. (2020a) prove that computing technical capacities, i.e., finding a feasible booking maximizing a weighted sum of the values at every node, is NP-hard, even on passive trees.

As previously discussed in Section 3.3, the results of [FP3] have already been used in Böttger et al. (2020) and Schewe et al. (2020b). Böttger et al. (2020) compute the cost of decoupling in the European entry-exit market, based on the four-level model of Grimm et al. (2019) and modeling gas physics by linear potential-based flows. Using nonlinear potential-based flows, Schewe et al. (2020b) solve the four-level model to global optimality on passive trees.

Checking the feasibility of a booking requires to assess that all booking-compliant nominations are feasible. As a consequence of the hardness result presented by

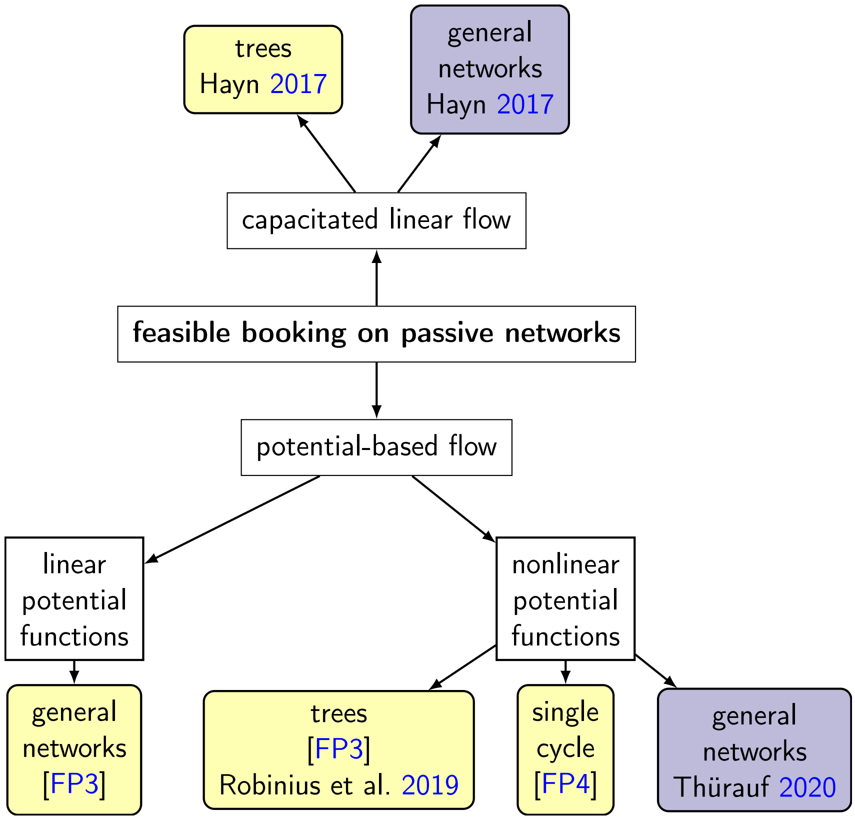

Figure 3.2: Main complexity results (light=P, dark=coNP-hard) for the feasibility of bookings on passive networks (adapted from [FP3] and Thürauf (2020)).

Szabó (2012), Hayn et al. (2015) argue that this task might be hopeless in practice. The authors develop decision-support tools for real-world usage by TSOs. These tools are of stochastic nature and heuristically check a booking for feasibility by verifying the feasibility of a significant, but finite, subset of booking-compliant nominations. In this dissertation, we study the feasibility of bookings in the robust sense (3.5). The set of booking-compliant nominations can be considered as an uncertainty set for the load flows to be transported on the network. Along these lines, the PhD thesis by Aßmann (2019) as well as the recent articles by Aßmann et al. (2018, 2019), treat gas transport under uncertainties from the point-of-view of two-stage robust optimization. Aßmann et al. (2018) discuss two-stage robust feasibility problems with an empty first stage, i.e., all variables are adjustable after the uncertainty realizes, and for which the constraints are given by polynomials. The authors first reformulate these problems as set containment problems. They then present two separate approaches to decide feasibility and infeasibility using tools from polynomial optimization. The authors apply their findings to the example of stationary gas transport in passive networks with uncertain physical parameters, i.e., the pipe-specific constants Λ in (3.4b). For tree-shaped networks, Aßmann et al. (2018) show that the robust feasibility can be decided efficiently by solving a polynomial number of LPs.

Aßmann et al. (2019) study cost-optimal and stationary gas transport in networks with linearly modeled compressors under uncertainties in the nomination and the physical parameters. In their setting, the TSO minimizes the (linear) cost of operating compressors, while accounting for uncertainties in the subsequent gas transport in a robust way, which results in a two-stage robust optimization problem. Aßmann et al. (2019) exploit the decomposable structure of the problem to derive a single-stage reformulation. Using the results by Aßmann et al. (2019) on passive networks particularly allows to decide the feasibility of a booking and these results are therefore closely related to our work in [FP3]. However, the techniques used in the two publications are very different. In addition, we also study networks with linearly modeled elements in [FP5]. The key difference to the work by Aßmann et al. (2019) is that, therein, the authors consider the controls of the active elements as "here-and-now" decisions, i.e., decisions that need to be fixed before the realizations of the uncertain nomination. In [FP5], we consider the dynamics faced by a TSO, when assessing the feasibility of bookings in the active case. In this setting, the TSO exploits all possibilities to guarantee the feasibility of booking-compliant nominations and controls the active elements individually for each nomination. In the view of two-stage robust optimization, the controls of the active elements are then also "wait-and-see" decisions, just like the flows and potentials, that can be adjusted to every nomination.

4

Feasibility of Bookings in the European Entry-Exit Gas Market

In this chapter, we present the main results of [FP3; FP4; FP5] on checking the feasibility of bookings. In Section 4.1, we discuss a characterization of feasible bookings on passive networks derived in [FP3]. Section 4.2 is then devoted to the special case of a passive network that is a tree. The results of [FP4] for a single-cycle network in the passive case are summarized in Section 4.3. Finally, we present the theoretical findings of [FP5] for the case of networks with linearly modeled active elements in Section 4.4 and the corresponding computational case study in Section 4.5.

To streamline the summary of these three publications, we adapt the results in [FP3] to use the notations and definitions presented in Chapter 3, and more importantly to match the common framework of [FP4; FP5]. Note, however, that all results presented in Sections 4.1 and 4.2 are mathematically equivalent to those in the respective publications. Also recall that in this dissertation, we do not consider bounds on the flows and they are therefore neglected during the presentation of [FP3].

4.1 General Passive Networks

In this section, we consider a weakly connected network $G = (V, A)$ without controllable elements, i.e., $A_{\text{act}} = \emptyset$ and $A = A_{\text{pipe}}$. In particular, only flows q and potentials π are required to define a potential-based flow satisfying (3.4), as Constraints (3.4c) and (3.4d) are not present. As seen in Proposition 3.3, the flows $q := q(\ell)$ in a potential-based flow uniquely correspond to a given nomination ℓ in passive networks. The same holds for potential differences $\pi_u - \pi_v$ on pipes $(u, v) \in A_{\text{pipe}}$. Furthermore, the potential π_w at any node $w \in V$ can be linked to π_o at an arbitrary reference node $o \in V$ by summing up the potential differences along an undirected path $P := P(o, w)$ connecting o to w in G. This then yields

$$\pi_w = \pi_o - \sum_{(u,v) \in A(P)} \eta_{(u,v)}(P)(\pi_u - \pi_v), \tag{4.1}$$

where $\eta_a(P)$ for an arc $a = (u, v) \in A(P)$ evaluates to 1, if a is directed from o to w along P, and to -1 otherwise. In particular, the potentials π at all nodes are uniquely determined by the nomination ℓ and the reference potential π_o, because

$$\pi_w = \pi_o - \sum_{a \in A(P(o,w))} \eta_a(P(o, w))\Lambda_a |q_a(\ell)| q_a(\ell), \quad w \in V, \tag{4.2}$$

holds by combining (3.4b) and (4.1). To determine the feasibility of nomination ℓ, in addition to computing the implicitly defined flows $q(\ell)$, it is required to find a reference potential π_o such that the resulting potentials do not violate the bounds in (3.4e). However, it directly follows from (4.2) that, in addition to pipes $(u, v) \in A_{\text{pipe}}$, the potential differences of every pair of nodes $(w_1, w_2) \in V^2$ is uniquely determined by the nomination ℓ and given by

$$\pi_{w_1} - \pi_{w_2} = \sum_{a \in A(P(w_1,w_2))} \eta_a(P(w_1, w_2))\Lambda_a |q_a(\ell)| q_a(\ell).$$

Theorem 1 in Gotzes et al. (2016) characterizes feasible nominations in passive networks in terms of the potential differences between all pairs of nodes and thus eliminates the dependence on the reference potential π_o. In [FP3], we derive the same result using an alternative proof, in which we replace the potentials in (3.4e) using (4.2) and then apply Fourier–Motzkin elimination to project out π_o.

Theorem 4.1 (Theorem 7 in [FP3])**.** *Let $G = (V, A)$ be a weakly connected and passive network. Then, the nomination $\ell \in N$ is feasible if and only if there exists a feasible point (q, π) of (3.4a) and (3.4b) such that $\pi_{w_1} - \pi_{w_2} \leq \pi^+_{w_1} - \pi^-_{w_2}$ holds for every pair of nodes $(w_1, w_2) \in V^2$.*

Instead of the bounds in (3.4e) on potentials at every node, we can thus equivalently consider bounds on potential differences as given in Theorem 4.1. The uniqueness of these potential differences in passive networks allows us to obtain a characterization of feasible bookings based on the result of Theorem 4.1 by optimizing over all booking-compliant nominations.

Theorem 4.2 (Theorem 10 in [FP3])**.** *Let $G = (V, A)$ be a weakly connected and passive network. 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 $(w_1, w_2) \in V^2$, where we define*

$$\phi_{w_1 w_2}(b) := \max_{\ell, q, \pi} \left\{ \pi_{w_1} - \pi_{w_2} \colon (3.4a), (3.4b), \ell \in N(b) \right\}. \tag{4.3}$$

Intuitively, the only free decision variable in Problem (4.3) is $\ell \in N(b)$, since flows and potential differences are uniquely determined as soon as a nomination is

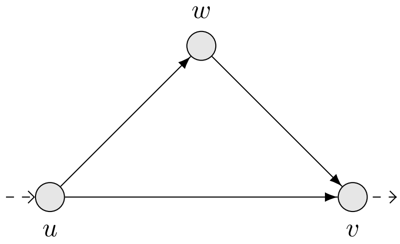

Figure 4.1: Network of Example 4.3.

given. Consequently, optimizing over q and π satisfying (3.4a) and (3.4b) is a way of implicitly computing a potential-based flow $(q(\ell), \pi)$ corresponding to ℓ. This is a notable difference to the studies of Hayn (2017) using capacitated linear flow models to represent gas transport, where a single-level formulation comparable to (4.3) is hardly adequate. As a consequence of the missing uniqueness of flows, the TSO has a free choice of the flows corresponding to a given load flow and would choose the best solution to minimize a violation of the technical restrictions. As a consequence, an appropriate model for that setting should emphasize the resulting max-min nature of the decision process. In Section 4.4, we will focus more on this aspect when considering potential-based flows with active elements, in which, for every load flow, the TSO has a free choice of the controls to apply to the active elements.

For a single nomination ℓ on a passive network, flows $q(\ell)$ can be computed by solving the strictly convex minimization problem given by Maugis (1977) and Collins et al. (1978) and the potentials π are obtained as corresponding dual solutions. The feasibility of ℓ can then be checked by Theorem 4.1. On the other hand, validating the feasibility of a booking on a passive network requires the solution of a nonlinear and nonconvex optimization problem for every pair of nodes $(w_1, w_2) \in V^2$. Thürauf (2020) proves that solving Problem (4.3) is NP-hard. If the right-hand sides of (3.4b) are replaced by linear functions of the flows, Problem (4.3) is an LP. Thus, when considering linear potential-based flows and passive networks, the feasibility of a booking can be decided in polynomial time; see [FP3]. However, for nonlinear potential-based flows (3.4), Thürauf (2020) shows that the problem is coNP-hard on passive networks. For the problem to also be in coNP, there has to be a certificate of infeasibility that can be checked in polynomial time. Furthermore, by definition of coNP, the encoding length of the certificate must be polynomial in the size of the input. In [FP3], we claim that checking the feasibility of a booking on passive networks with nonlinear potential-based flows is in coNP. The certificate given in our proof contains, besides the infeasible nomination, its corresponding flows. However, even if all input data are rational, the flows corresponding to an infeasible nomination could be irrational, as shown in the following example.

Example 4.3. Consider the passive network shown in Figure 4.1, given by

$$G = (V = \{u, v, w\}, A = \{(u, v), (u, w), (w, v)\}),$$

where the nodes are partitioned into $V_+ = \{u\}$, $V_- = \{v\}$, and $V_0 = \{w\}$. Let

$\Lambda_a = 1$ for all $a \in A$ and the nomination ℓ is given by $\ell_u = \ell_v = 1$ and $\ell_w = 0$. This construction implies that $q_a \geq 0$ holds for all $a \in A$. By the flow conservation constraints (3.4a), we observe that

$$q_{(u,w)} = q_{(w,v)}, \quad q_{(u,w)} + q_{(u,v)} = 1, \quad q_{(w,v)} + q_{(u,v)} = 1$$

hold. Additionally, (3.4b) implies that the potential difference between u and v must be the same, independent of whether it is computed via w or directly, i.e.,

$$\pi_u - \pi_v = |q_{(u,v)}|q_{(u,v)} = |q_{(u,w)}|q_{(u,w)} + |q_{(w,v)}|q_{(w,v)}$$

is satisfied. Since flows are nonnegative, we thus derive the following system of equations

$$q_{(u,v)} = \sqrt{2}q_{(u,w)}, \quad q_{(u,v)} = 1 - q_{(u,w)}, \quad q_{(w,v)} = q_{(u,w)},$$

whose solution is given by

$$q_{(u,v)} = \frac{\sqrt{2}}{1+\sqrt{2}}, \quad q_{(u,w)} = q_{(w,v)} = \frac{1}{1+\sqrt{2}}.$$

The encoding length of the certificate of infeasibility presented in [FP3] is thus not polynomial in the input size in general. This "proof" does not allow to conclude that the problem is in coNP. However, it does neither affect the hardness result of Thürauf (2020) nor the polynomial cases investigated in [FP3; FP4]. Furthermore, a certificate of polynomial size might still exist for the general passive case with nonlinear potential-based flows. As a consequence of the previous example, such a certificate must not be given in terms of possibly irrational flows. Note also that for capacitated linear flows, the problem is indeed shown to be coNP-complete by Hayn (2017). In this case, computing flows does not require taking roots, in contrast to nonlinear potential-based flows, and thus rational input data lead to rational flows.

4.2 Passive Tree-Shaped Networks

In [FP3], we additionally show that for passive trees the nonlinear and nonconvex optimization problems (4.3) can be solved efficiently. Therefore, consider a passive tree $T = (V, A)$ with $A = A_{\text{pipe}}$. We assume w.l.o.g. that T is a rooted out-tree with root $o \in V$. If the latter were not the case, we could transform every feasible potential-based flow by simply switching the sign of flows along wrongly directed arcs. Figure 4.2 shows an example of passive tree network with root o.

The rooted tree structure allows us to consider subtrees in T. Let $T(u)$ denote the subtree rooted in a node $u \in V$. In particular, $T = T(o)$ holds. On the tree T, we give an explicit and closed-form formula for $q(\ell)$. Flow conservation constraints (3.4a) fully determine flows on a tree w.r.t. the nomination ℓ. Intuitively, the total offer or demand of a subtree rooted in a node v must traverse the incident arc (u, v). Thus, for an arc $(u, v) \in A$, the flow is given by

$$q_{(u,v)}(\ell) = \sum_{v' \in V_- \cap V(T(v))} \ell_{v'} - \sum_{v' \in V_+ \cap V(T(v))} \ell_{v'}.$$

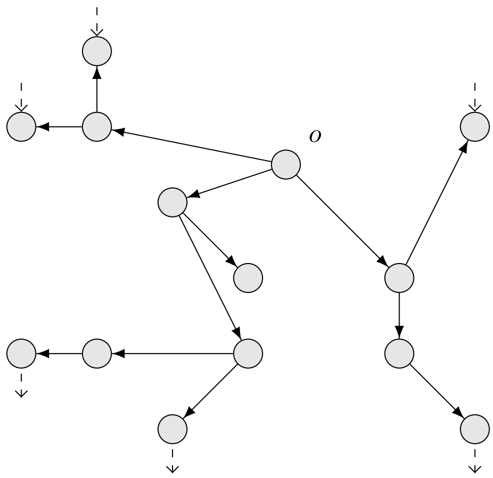

Figure 4.2: Example of a passive tree with all arcs directed away from the root o (adapted from [FP5]).

Consequently, if we let $P(o,u)$ denote the unique and directed path in T from o to $u \in V$, then it follows by (4.2) that

$$\pi_u = \pi_o - \sum_{a \in A(P(o,u))} \Lambda_a |q_a(\ell)| q_a(\ell).$$

The potential difference of a pair of nodes $(w_1, w_2) \in V^2$ is then also given as a function of ℓ, since

$$\pi_{w_1} - \pi_{w_2} = - \sum_{a \in A(P(w,w_1))} \Lambda_a |q_a(\ell)| q_a(\ell) + \sum_{a \in A(P(w,w_2))} \Lambda_a |q_a(\ell)| q_a(\ell)$$

holds, where $w \in V$ is the last common node of $P(o, w_1)$ and $P(o, w_2)$, i.e., the first common ancestor of w_1 and w_2 in T.

Exploiting the monotonicity of the function $f(x) = |x|x$, Problem (4.3) is cast as a sequence of knapsack problems with continuous variables and can be solved by dynamic programming.[1] Then, the optimal value in (4.3) for a pair of nodes $(w_1, w_2) \in V^2$ is obtained by sending the maximum amount of flow possible w.r.t. the booking b from w_1 to w_2. More precisely, we have the following theorem.

[1] Note that the formulas in Lemma 17 in [FP3] for an arc $(u, v) \in A$ should read

$$\max_{q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})} \Phi_{uv} \left(\sum_{l \in V(T(v))} q_l^{\mathrm{n}} \right) = \Phi_{uv} \left(\min \left\{ \sum_{k \in V_- \setminus V(T(v))} q_k^{\mathrm{b}}, \sum_{k \in V_+ \cap V(T(v))} q_k^{\mathrm{b}} \right\} \right)$$

and

$$\min_{q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})} \Phi_{uv} \left(\sum_{l \in V(T(v))} q_l^{\mathrm{n}} \right) = -\Phi_{uv} \left(\min \left\{ \sum_{k \in V_+ \setminus V(T(v))} q_k^{\mathrm{b}}, \sum_{k \in V_- \cap V(T(v))} q_k^{\mathrm{b}} \right\} \right).$$

Theorem 4.4 (Corollary 19 in [FP3]). *Let T be a passive tree and $b \in L$ be a booking. Then,*

$$\phi_{w_1 w_2}(b) = -\sum_{a \in A(P(w,w_1))} \Lambda_a |\underline{q}_a| \underline{q}_a + \sum_{a \in A(P(w,w_2))} \Lambda_a |\overline{q}_a| \overline{q}_a$$

holds for every pair of nodes $(w_1, w_2) \in V^2$, where $w \in V$ is the last common node of $P(o, w_1)$ and $P(o, w_2)$ and for every $(u, v) \in A$, we define

$$\underline{q}_{(u,v)} := -\min\left\{ \sum_{v' \in V_+ \cap V(T(v))} b_{v'}, \sum_{v' \in V_- \setminus V(T(v))} b_{v'} \right\},$$

$$\overline{q}_{(u,v)} := \min\left\{ \sum_{v' \in V_- \cap V(T(v))} b_{v'}, \sum_{v' \in V_+ \setminus V(T(v))} b_{v'} \right\}.$$

In Theorem 4.4, the maximum potential difference w.r.t. the booking b is reached by sending the minimum amount of flow $\underline{q}$ along $P(w, w_1)$ and the maximum amount of flow $\overline{q}$ along $P(w, w_2)$. Therein, the minimum amount of flow corresponds in fact to the maximum amount of flow that can be sent against the arc direction. Using Theorem 4.4, maximum potential differences on a tree can be computed in polynomial time. It remains to check the inequalities of Theorem 4.2 to assess the feasibility of b, which leads to the following result.

Theorem 4.5 (Theorem 20 in [FP3]). *Verifying the feasibility of a booking $b \in L$ on passive trees is in* P.

Given the tree structure of the network, it is possible to efficiently compute flows that lead to a maximum potential difference between a pair of nodes. On trees, it is therefore possible to solve the nonlinear and nonconvex problems (4.3) for every $(w_1, w_2) \in V^2$. In the absence of cycles, flows are uniquely determined by the flow conservation constraints (3.4a). There is no split of flows along multiple paths, which would have to be resolved by Constraints (3.4b). Consequently, the flows in an optimal solution of (4.3) are rational whenever the booking is rational. This is in contrast to the situation observed in Example 4.3, but can clearly be seen in (4.4). The easiest class of passive networks in which flows split along more than one path are single-cycle networks. Since the rank of the flow conservation constraints is $|V| - 1$, there is now one flow variable that is determined by (3.4b). In the next section, we analyze the structure of nominations and flows that lead to maximum potential differences on a passive cycle. In doing so, we are able to sufficiently reduce the dimension of Problem (4.3), which allows us to efficiently apply general decision algorithms from real algebraic geometry to decide the feasibility of a booking.

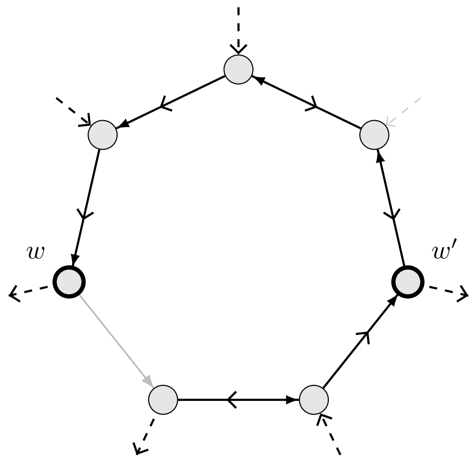

Figure 4.3: Entry-exit activity and flow directions (bold arcs) along an exemplary cycle and resulting flow-meeting points w and w' (taken from [FP4]).

4.3 Passive Single-Cycle Networks

In [FP4], we study a passive network $G = (V, A)$ that consists of a single cycle and show that the characterization of Theorem 4.2 can still be checked in polynomial time. To do so, we first analyze the structure of optimal solutions of Problem (4.3) for any pair of nodes $(w_1, w_2) \in V^2$.

On a cycle, for every pair of nodes $(o, w) \in V^2$, there are exactly two undirected paths between o and w in G. The "left" path, joining o to w in counter-clockwise direction, is denoted by $P^{\mathrm{l}}(o, w)$. The "right" path, joining o to w in clockwise direction, is denoted by $P^{\mathrm{r}}(o, w)$. Recall that if P denotes any of the two paths, then $\eta_a(P)$ evaluates to 1 if arc $a = (u, v) \in A(P)$ is directed from o to w along P, and to -1 otherwise. By Constraints (3.4b), the potential difference between o and w is the same, independently of the path along which it is computed. More precisely,

$$\pi_o - \pi_w = \sum_{a \in A(P^{\mathrm{l}}(o,w))} \eta_a(P^{\mathrm{l}}(o, w)) \Lambda_a |q_a| q_a = \sum_{a \in A(P^{\mathrm{r}}(o,w))} \eta_a(P^{\mathrm{r}}(o, w)) \Lambda_a |q_a| q_a$$

holds. Thus, there cannot be cycling flow on G, as it would lead to mismatching potentials before and after passing all arcs of the cycle. Consequently, flows have to "meet" at least once along the cycle G. In [FP4], we formalize this notion using so-called flow-meeting points. Here, we simply refer to Figure 4.3 to convey some intuition. Bold arcs indicate the entry-exit activity for a given nomination as well as the directions of the corresponding flows. In contrast, grayed out arcs represent inactive entries or exits and arcs with zero flow. For a given nonzero nomination, a flow-meeting point is therefore a special exit, reached by a nonnegative amount of flow along both incident arcs. To break ties, we ensure that zero flow is always to the right of a flow-meeting point; see the node w.

Given the monotonicity of the function $f(x) = |x|x$, it is possible to observe that, the more flows change directions along the cycle G, the smaller the overall potential loss is in G. In particular, when solving Problem (4.3) for a pair of nodes $(w_1, w_2) \in V^2$, fewer flow-meeting points result in a larger potential difference $\pi_{w_1} - \pi_{w_2}$.

Theorem 4.6 (Theorem 12 in [FP4]). *Let $G = (V, A)$ be a passive cycle and $b \in L$ be a booking. Then, for a fixed pair of nodes $(w_1, w_2) \in V^2$, there exists an optimal solution of Problem (4.3) that has at most one flow-meeting point $w \in V_-$.*

Note that every nonzero nomination admits at least one flow-meeting point, since flows must change directions in a cycle. If a nonzero nomination admits exactly one flow-meeting point w, there exists an entry $o \in V_+$ with highest potential from which a nonnegative amount of flow travels to w along both paths in G. Observe that consequently, the exit and flow-meeting point w has the lowest potential. This is summarized in the following result.

Corollary 4.7 (Corollary 13 in [FP4]). *Let $G = (V, A)$ be a passive cycle and $b \in L$ be a booking. Then, for a fixed pair of nodes $(w_1, w_2) \in V^2$, there exist a pair of nodes $(o, w) \in V_+ \times V_-$ and an optimal solution (ℓ, q, π) of Problem (4.3) such that $q_a \geq 0$ holds for every $a \in A'$. Here, A' is obtained from A by orienting all arcs such that $P^{\mathrm{l}}(o, w)$ and $P^{\mathrm{r}}(o, w)$ are directed paths in G.*

Recall that in potential-based flows, the direction of pipes serves to interpret the sign of flows in G. By reorienting the arcs, we do not modify the problem, because all feasible solutions can be mapped to each other by equally changing the sign of the corresponding flows. Corollary 4.7 implies that, for every pair of nodes $(w_1, w_2) \in V^2$, the feasible domain of Problem (4.3) can be restricted by considering all pairs $(o, w) \in V_+ \times V_-$ and nonnegative flows from o to w. We thus derive the following characterization of feasible bookings on a single cycle.

Theorem 4.8 (Corollary 15 in [FP4]). *Let $G = (V, A)$ be a passive cycle. Then, the booking $b \in L$ is feasible if and only if $\bar{\varphi}^{ow}_{w_1 w_2}(b) \leq \pi^+_{w_1} - \pi^-_{w_2}$ holds for all pairs of nodes $(w_1, w_2) \in V^2$ and $(o, w) \in V_+ \times V_-$, where we define*

$$
\begin{aligned}
\bar{\varphi}^{ow}_{w_1 w_2}(b) := \max_{\ell, q, \pi} \quad & \pi_{w_1} - \pi_{w_2} && \text{(4.4a)} \\
\text{s.t.} \quad & \text{(3.4a)}, \ \ell \in N(b), \\
& \pi_u - \pi_v = \Lambda_a |q_a| q_a, \quad a = (u, v) \in A', && \text{(4.4b)} \\
& q_a \geq 0, \quad a \in A'. && \text{(4.4c)}
\end{aligned}
$$

As a consequence, a booking is infeasible if and only if there are two pairs of nodes $(w_1, w_2) \in V^2$ and $(o, w) \in V_+ \times V_-$ such that

$$\pi_{w_1} - \pi_{w_2} > \pi^+_{w_1} - \pi^-_{w_2}, \ \text{(3.4a)}, \ \ell \in N(b), \ \text{(4.4b)}, \ \text{(4.4c)}, \tag{4.5}$$

admits a solution. Additionally, since $q_a \geq 0$ holds for all $a \in A'$, the right-hand sides of (4.4b) are equivalent to q_a^2. Checking the feasibility of a booking on a passive cycle is thus reduced to finding a solution to a system of polynomial equations and inequalities of degree at most two. As such, it may be seen as a general quantifier elimination problem from real algebraic geometry; see the book by Basu et al. (2007). These problems are often studied for their parametric complexity and admit algorithms that are doubly exponential in the problem size. Here, we aim to reduce the system of polynomials to a constant number of variables, equations, and inequalities, that is independent of the size of the cycle. In this case, a quantifier elimination procedure can be used as an efficient oracle in an algorithm to assess the feasibility of a booking on single passive cycles.

Let now $(w_1, w_2) \in V^2$ and $(o, w) \in V_+ \times V_-$ be given and fixed. In this dissertation, we focus on the structural analysis in [FP4] of solutions of Problem (4.4) if $w_1, w_2 \in V(P^{\mathrm{r}}(o, w))$. Since this case leads to a larger number of variables and constraints in the reduced system of polynomials, it determines the complexity results. For details on the case in which w_1 and w_2 lie on two different paths w.r.t. o and w, we refer to [FP4]. To be able to discuss the order of nodes $u, v \in V(P^{\mathrm{r}}(o, w))$, we denote $u \prec_{\mathrm{r}} v$ if u precedes v when moving from o to w along $P^{\mathrm{r}}(o, w)$. Additionally, $u \preceq_{\mathrm{r}} v$ is a shortcut for $u \prec_{\mathrm{r}} v$ or $u = v$. Similarly, we introduce the notations $u \prec_{\mathrm{l}} v$ and $u \preceq_{\mathrm{l}} v$ for $u, v \in V(P^{\mathrm{l}}(o, w))$.

Considering the feasibility of a booking on passive networks, it is natural to assume that the zero nomination is always feasible, since it complies with every booking. In order to ship the zero nomination, i.e., zero flow, the potentials at all nodes in the network need to be fixed to the same constant. For this to be possible, we make the following assumption.

Assumption 4.9. $\pi^+_{w_1} \geq \pi^-_{w_2}$ holds for every pair of nodes $(w_1, w_2) \in V^2$.

In particular, this allows us to only consider $w_1 \prec_{\mathrm{r}} w_2$. As a consequence of the nonnegative flows, the optimal value of Problem (4.4) is always nonpositive for $w_2 \preceq_{\mathrm{r}} w_1$ and can thus not lead to an infeasible nomination w.r.t. the characterization of Theorem 4.8. In solving Problem (4.4), the goal is to find a nomination that leads to a maximum potential difference between w_1 and w_2. From that point of view, it is possible to further reduce the feasible domain of (4.4) to only take into account nominations that exploit the booking with a certain structure.

Theorem 4.10 (Theorem 35 in [FP4])**.** *There exist entries $s^{\mathrm{l}}_1, s^{\mathrm{l}}_2, s^{\mathrm{r}}_1, s^{\mathrm{r}}_2 \in V_+$, exits $t^{\mathrm{l}}_1, t^{\mathrm{r}}_1, t^{\mathrm{r}}_2 \in V_-$, and an optimal solution of Problem (4.4) such that the following additional properties are satisfied.*

(a) $s^{\mathrm{l}}_1, s^{\mathrm{l}}_2 \in V_+ \cap V(P^{\mathrm{l}}(o, w))$ *with* $s^{\mathrm{l}}_1 \preceq_{\mathrm{l}} s^{\mathrm{l}}_2$ *and for every entry* $v \in V_+ \cap V(P^{\mathrm{l}}(o, w))$*, it holds*

$$\ell_v = \begin{cases} 0, & \text{if } o \prec_{\mathrm{l}} v \prec_{\mathrm{l}} s^{\mathrm{l}}_1 \text{ or } s^{\mathrm{l}}_2 \prec_{\mathrm{l}} v \prec_{\mathrm{l}} w, \\ b_v, & \text{if } s^{\mathrm{l}}_1 \prec_{\mathrm{l}} v \prec_{\mathrm{l}} s^{\mathrm{l}}_2. \end{cases}$$

(b) $t^{\mathrm{l}}_1 \in V_- \cap V(P^{\mathrm{l}}(o, w))$ *and for every exit* $v \in V_- \cap V(P^{\mathrm{l}}(o, w))$*, it holds*

$$\ell_v = \begin{cases} 0, & \text{if } o \prec_{\mathrm{l}} v \prec_{\mathrm{l}} t^{\mathrm{l}}_1, \\ b_v, & \text{if } t^{\mathrm{l}}_1 \prec_{\mathrm{l}} v \preceq_{\mathrm{l}} w. \end{cases}$$

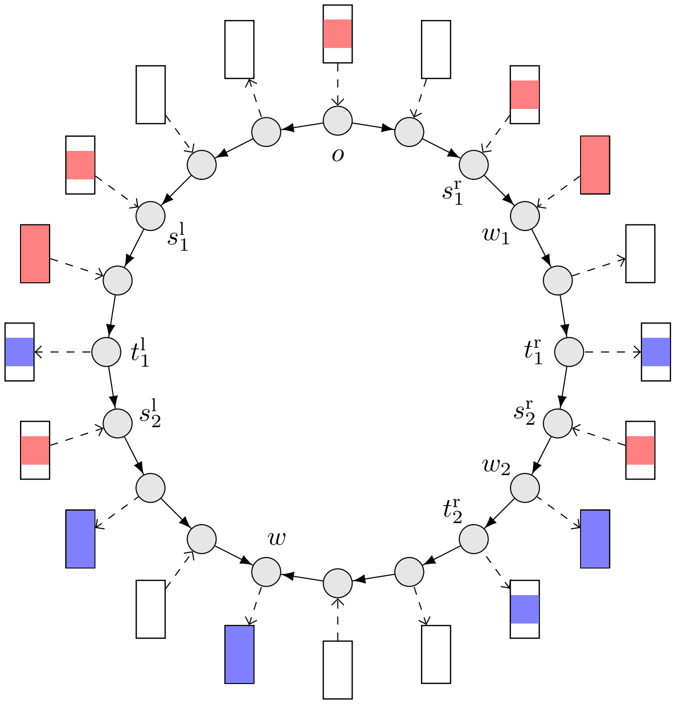

Figure 4.4: Configuration of s and t nodes with $o \preceq_{\mathrm{r}} w_1 \prec_{\mathrm{r}} w_2 \preceq_{\mathrm{r}} w$ (taken from [FP4]).

(c) $s_1^{\mathrm{r}}, s_2^{\mathrm{r}} \in V_+ \cap V(P^{\mathrm{r}}(o,w))$ *with* $s_1^{\mathrm{r}} \preceq_{\mathrm{r}} s_2^{\mathrm{r}}$ *and for every entry* $v \in V_+ \cap V(P^{\mathrm{r}}(o,w))$, *it holds*

$$\ell_v = \begin{cases} 0, & \text{if } o \prec_{\mathrm{r}} v \prec_{\mathrm{r}} s_1^{\mathrm{r}} \text{ or } s_2^{\mathrm{r}} \prec_{\mathrm{r}} v \prec_{\mathrm{r}} w, \\ b_v, & \text{if } s_1^{\mathrm{r}} \prec_{\mathrm{r}} v \prec_{\mathrm{r}} s_2^{\mathrm{r}}. \end{cases}$$

(d) $t_1^{\mathrm{r}}, t_2^{\mathrm{r}} \in V_- \cap V(P^{\mathrm{r}}(o,w))$ *with* $t_1^{\mathrm{r}} \preceq_{\mathrm{r}} t_2^{\mathrm{r}}$ *and for every exit* $v \in V_- \cap V(P^{\mathrm{r}}(o,w))$, *it holds*

$$\ell_v = \begin{cases} 0, & \text{if } o \prec_{\mathrm{r}} v \prec_{\mathrm{r}} t_1^{\mathrm{r}} \text{ or } t_2^{\mathrm{r}} \prec_{\mathrm{r}} v \prec_{\mathrm{r}} w, \\ b_v, & \text{if } t_1^{\mathrm{r}} \prec_{\mathrm{r}} v \prec_{\mathrm{r}} t_2^{\mathrm{r}}. \end{cases}$$

Figure 4.4 shows an arrangement of the nodes $s_1^{\mathrm{l}}, s_2^{\mathrm{l}}, s_1^{\mathrm{r}}, s_2^{\mathrm{r}} \in V_+$ and $t_1^{\mathrm{l}}, t_1^{\mathrm{r}}, t_2^{\mathrm{r}} \in V_-$ as well as a representation of a nomination satisfying the properties of Theorem 4.10. Therein, boxes qualitatively illustrate the amount of the booking that is nominated. For $v \in V$, an empty box indicates that $\ell_v = 0$ and a full box that $\ell_v = b_v$. Note that for a given configuration, most of the nomination values are fixed, either to zero or the booking at a given node. Theorem 4.10 does however not restrict the nomination at nodes $s_1^{\mathrm{l}}, s_2^{\mathrm{l}}, s_1^{\mathrm{r}}, s_2^{\mathrm{r}}, t_1^{\mathrm{l}}, t_1^{\mathrm{r}}, t_2^{\mathrm{r}}$, and o. We have seen in Section 4.2 that on trees, flows are explicitly expressible as a function of the nomination. On a cycle, on the contrary, there is one arc flow that cannot be obtained only by the flow conservation constraints (3.4a). Thus, an optimal solution of Problem (4.4) on a cycle is defined by nine variables, independently of the size of the cycle. More precisely, the following result holds.

Theorem 4.11 (Theorem 39 in [FP4]). *Let $(w_1, w_2) \in V^2$ and $(o, w) \in V_+ \times V_-$ be fixed pairs of nodes. Then, System (4.5) can equivalently be rewritten as a system of polynomial equations and inequalities of degree at most two and with at most nine variables and 42 constraints.*

As previously discussed, a general decision algorithm, such as Algorithm 14.16 in Basu et al. (2007), can be applied to efficiently determine the existence of a solution to the resulting constant-size system of polynomials. Iterating this procedure over $(w_1, w_2) \in V^2$, $(o, w) \in V_+ \times V_-$, $s_1^{\mathrm{l}}, s_2^{\mathrm{l}}, s_1^{\mathrm{r}}, s_2^{\mathrm{r}} \in V_+$, and $t_1^{\mathrm{l}}, t_1^{\mathrm{r}}, t_2^{\mathrm{r}} \in V_-$ yields the final complexity result for passive single-cycle networks.[2]

Theorem 4.12 (Corollary 41 in [FP4]). *Verifying the feasibility of a booking $b \in L$ on single passive cycles is in* P*.*

Note that on a cycle, flows corresponding to a rational nomination might be irrational, as shown in Example 4.3. However, Algorithm 14.16 in Basu et al. (2007) never actually computes any flows. Intuitively, a general decision algorithm for a system of equations and inequalities successively projects out variables until the space of solutions is either detected to be empty or there remain no more variables. The procedure described in this section can therefore assess the feasibility of a booking, it does, however, not produce the worst-case nomination and its corresponding flows and potentials.

Up to this point, we have observed that checking the feasibility of a booking on general passive networks is a hard task; see Thürauf (2020). On passive trees and cycles, we have presented two algorithms to decide the problem in polynomial time. While our approach for trees is rather straightforward, the analysis of the cycle requires an extensive combinatorial study of the structure of solutions of Problem (4.3). Although, the study of the cycle provides significant structural insights, the presented algorithm is more of a theoretical nature. More general classes of passive networks might be tackled by a combination of the techniques applied for trees and single cycles. Such studies would, however, mostly benefit the theoretical quest for the frontier of hardness, i.e., finding the most general class of passive networks for which deciding the feasibility of a booking is still polynomial. In practice, Problem (4.3) can be solved using global optimization solvers, such as BARON or ANTIGONE. Furthermore, most realistic networks, if not all, contain some form of active elements. They provide the TSO with some flexibility in transporting gas through the network, whereas the TSO has no influence on gas flows in the passive case. In the next section, we thus directly turn to active networks and extend the characterization of feasible bookings presented in Section 4.1. We present bilevel models for the feasibility of a booking, taking into account the fact that the TSO can now actively react to every nomination.

[2] Note that an additional factor of $|V|^2$ is required in the complexity of Corollary 41 in [FP4] to account for the iterations over $(w_1, w_2) \in V^2$.

4.4 Networks with Linearly Modeled Active Elements

We now turn to the feasibility of bookings on networks with active elements and modeled by potential-based flows (3.4). Consider an active network $G = (V, A)$ with linearly modeled compressors $A_{\text{cm}} \subseteq A$ and control valves $A_{\text{cv}} \subseteq A$. In contrast to the passive case, the TSO is now able to influence gas flows corresponding to a given nomination. Individually for every nomination $\ell \in N(b)$, the TSO uses the active elements to control the transport of the nominated amounts within the limitations of the network. In Section 3 of [FP5], a small example is discussed showing that a single-level approach, like the characterization of Theorem 4.2 for passive networks, does not apply when considering active networks. In addition, the set of feasible nominations, shown to be connected for passive networks by Schewe et al. (2020c), may now be disconnected due to the discontinuity in operation of active elements, modeled by the indicator functions χ_a and Constraints (3.4d) for $a \in A_{\text{act}}$. The monotonic relation that more flow between two nodes implies a larger potential difference does not hold anymore. Under a certain threshold of flow on an arc $a \in A_{\text{act}}$, the active element is in bypass mode, i.e., $\Delta_a = 0$, resulting in a possibly larger potential difference. In this case, the TSO is unable to use the element to compensate for the potential loss caused by the nomination.

In [FP5], we present a bilevel optimization approach to decide the feasibility of a booking on active networks. Bilevel optimization allows to model the adversarial interplay of a worst-case nomination player and the TSO. The upper-level player chooses the worst booking-compliant nomination w.r.t. the violation of potential bounds. The lower-level player, i.e., the TSO, determines flows, potentials, and controls of the active elements to minimize the violation. This structure leads to the following result.

Theorem 4.13 (Proposition 4.1 in [FP5])**.** *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*

$$\begin{aligned}
\sup_{\ell \in N(b)} \ \min_{q,\pi,\Delta,y,z} \quad & y + z && \text{(4.6a)}\\
\text{s.t.} \quad & \text{(3.4a)–(3.4d)}, \\
& \pi_u + y \geq \pi_u^-, \quad u \in V, && \text{(4.6b)}\\
& \pi_u - z \leq \pi_u^+, \quad u \in V, && \text{(4.6c)}
\end{aligned}$$

admits a nonpositive optimal value.

Note the use of “sup” instead of “max”. As previously discussed in Section 2.1, the optimal solution of a bilevel problem might not be attained if there exist continuous linking variables (here, the nomination ℓ) and discrete decisions at the lower level (here, in the form of indicator functions χ). However, we will soon see that under a certain structural assumption, the bilevel problem can be reformulated such that the optimal solution is attained. In Problem (4.6), the leader chooses a nomination $\ell \in N(b)$ maximizing the total violation, i.e., the sum of the violation $y \in \mathbb{R}$ of lower

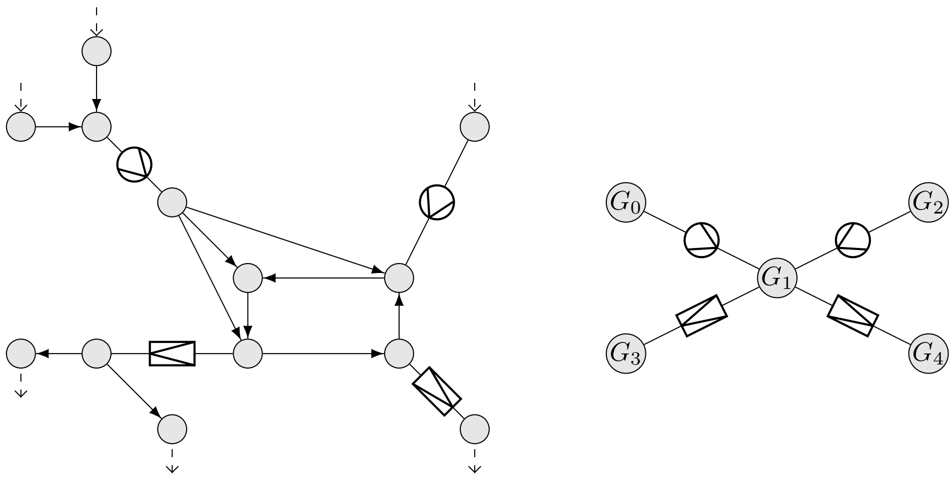

Figure 4.5: Active network satisfying Assumption 4.14 (left) and its corresponding reduced network (right) (taken from [FP5]).

potential bounds and the violation $z \in \mathbb{R}$ of upper potential bounds. The TSO, acting as the follower, determines a potential-based flow solving (3.4), with the only difference that $\pi_u \in [\pi_u^- - y, \pi_u^+ + z]$ must hold for every $u \in V$. Here, extending the potential bounds by y and z allows us to measure the violation corresponding to the leader's nomination. If $y > 0$, there exists a node such that its lower potential bound is violated. Otherwise, if $y \leq 0$, the nomination ℓ can be transported without violating any lower potential bounds. A similar interpretation holds for z and the violation of upper potential bounds. Consequently, if the optimal value of Problem (4.6) is nonpositive, all booking-compliant nominations are feasible and the booking is thus feasible. Problem (4.6) determines the worst-case nomination and, if applicable, the violation of potential bounds that corresponds to it. This is similar to the goal of the subproblems of the characterization of Theorem 4.2 for passive networks. However, on active networks, the TSO is allowed to react, since the potential-based flow can be influenced by the control of active elements.

Szabó (2012) shows that the feasibility of a nomination is already hard to decide on active networks. Consequently, doing so for bookings is even more challenging. Problem (4.6) is a bilevel model with linear upper level and a nonlinear and nonconvex lower level. In particular, the KKT reformulation, presented in Section 2.2, cannot be applied to (4.6). Furthermore, the presence of binary decisions in the form of indicator functions at the lower level, renders the bilevel problem very difficult; see Köppe et al. (2010). In an effort to gain some tractability, we make the following assumption on the placement of active elements, also considered by Borraz-Sánchez et al. (2016), Aßmann et al. (2019), and in the PhD thesis by Aßmann (2019).

Assumption 4.14. No active element is part of an undirected cycle in G.

This assumption is equivalent to assuming that the reduced network, defined by

Ríos-Mercado et al. (2002) and obtained by contracting all passive subnetworks into single nodes, is a tree. Figure 4.5 shows a network satisfying Assumption 4.14 on the left and its corresponding reduced network on the right. The reduced network is given by $\tilde{G} = (\mathcal{G}, A_{\text{act}})$, where $\mathcal{G} := \{G_0, G_1, \dots, G_{|A_{\text{act}}|}\}$ is the collection of passive subnetworks obtained by removing all active elements from G. For convenience, we 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 $v \in V(G_j)$.

Considering the networks presented in the GasLib (Schmidt et al. 2017), this assumption does not reflect reality in many cases. Active elements in a cycle would allow to send flow along that cycle, which is not possible in the passive case. The potential loss incurred along the cycle would lead to mismatching potentials at the beginning and end of the cycle. This effect could be countered by sufficiently increasing potentials in active elements along the cycle. From the point of view of cost, especially for the compression of gas, such a cycling flow situation is not realistic; see also the discussion around Figure 2.3 by Aßmann (2019). However, the feasibility of bookings is defined independently of costs. It would be possible to explicitly eliminate cycle flows using acyclic flow inequalities developed by Habeck and Pfetsch (2021). However, this approach would result in even more challenging models, that are out of the scope of this dissertation. Assumption 4.14 is a simpler means of eliminating cycle flows. It allows us to prove the uniqueness of flows corresponding to a nomination and thus extending this property of potential-based flows on passive networks.

Theorem 4.15 (Theorem 4.2 in [FP5])**.** *Let $G = (V, A)$ be a weakly connected network and suppose that Assumption 4.14 holds. Then, for a given nomination $\ell \in N$, every feasible point (q, π) of (3.4a) and (3.4b) admits the same unique flows $q(\ell)$ and potential differences $\pi_u - \pi_v$ are unique for all $(u, v) \in A_{\text{pipe}}$.*

For passive networks, this result is given by Proposition 3.3 and is derived from the studies of Maugis (1977), Collins et al. (1978), and Ríos-Mercado et al. (2002). Flows are thus already uniquely determined for nominations on the passive subnetworks of G. The tree structure of the reduced network $\tilde{G}$ allows us to additionally determine flows along active arcs A_{act}. As a consequence of this uniqueness, many of the physical quantities in the TSO's problem at the lower level are already fixed once a nomination is given by the upper-level player. For passive networks, all potentials π solving the System (3.4a) and (3.4b) are equivalent up to a constant shift. As a consequence of Theorem 4.15, this observation can now be extended to networks satisfying Assumption 4.14 by considering one shift per passive subnetwork $G_j \in \mathcal{G}$. More precisely, $\pi_u = \pi_u(\ell) + \tau_j$ holds for every node $u \in V(G_j)$ and every passive subnetwork $G_j \in \mathcal{G}$. Here, $\pi(\ell)$ is any solution of the System (3.4a) and (3.4b) with active elements in bypass mode, i.e., $\pi_u = \pi_v$ for all $(u, v) \in A_{\text{act}}$, and $\tau_j \in \mathbb{R}$ is a constant shift for the potentials in G_j. Active elements allow to include a potential change in between two passive subnetworks and the corresponding shifts are linked via (3.4c). Moving quantities that are already determined by physics to the upper level, we recast the bilevel problem (4.6) to only include the free decisions taken by the TSO at the lower level.

Theorem 4.16 (Theorem 4.3 in [FP5])**.** *Consider the bilevel problem*

$$
\begin{aligned}
\max_{\ell,q,\pi,s} \quad & y + z && \text{(4.7a)}\\
\text{s.t.} \quad & \text{(3.4a)}, \text{(3.4b)}, && \text{(4.7b)}\\
& \ell \in N(b), && \text{(4.7c)}\\
& \pi_u = \pi_v, \quad (u,v) \in A_{\text{act}}, && \text{(4.7d)}\\
& q_a \le m_a(1 - s_a) + M s_a, \quad a \in A_{\text{act}}, && \text{(4.7e)}\\
& s_a \in \{0,1\}, \quad a \in A_{\text{act}}, && \text{(4.7f)}\\
& (\Delta, \tau, y, z) \in \mathcal{S}(\ell, q, \pi, s), && \text{(4.7g)}
\end{aligned}
$$

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* $\mathcal{S}(\ell, q, \pi, s)$ *is given by*

$$
\begin{aligned}
\operatorname*{arg\,min}_{\Delta,\tau,y,z} \quad & y + z && \text{(4.8a)}\\
\text{s.t.} \quad & \tau_i - \tau_j = \begin{cases} -\Delta_a, & a = (G_i, G_j) \in A_{\text{cm}},\\ \Delta_a, & a = (G_i, G_j) \in A_{\text{cv}}, \end{cases} && \text{(4.8b)}\\
& \Delta_a \in [0, \Delta_a^+ s_a], \quad a \in A_{\text{act}}, && \text{(4.8c)}\\
& \tau_j + y \ge \pi_u^- - \pi_u, \quad u \in V(G_j),\ G_j \in \mathcal{G}, && \text{(4.8d)}\\
& \tau_j - z \le \pi_u^+ - \pi_u, \quad u \in V(G_j),\ G_j \in \mathcal{G}. && \text{(4.8e)}
\end{aligned}
$$

Under Assumption 4.14, Problems (4.6) and (4.7) admit the same optimal value.

Note that in Problem (4.7), the optimal solution is indeed attained as the lower level is only comprised of continuous variables, thus the use of "max". Consequently, for networks satisfying Assumption 4.14, the same holds for Problem (4.6) and in that case the "sup" is in fact a "max". In Problem (4.7), the leader is given the decision of all the physical quantities that are uniquely determined by the nomination. To this end, the leader determines, in addition to a worst-case nomination, a potential-based flow in G with bypassed active elements. The follower, i.e., the TSO, then optimally reacts by using the active elements and determining the corresponding shifts for each passive subnetwork. Observe that this is only possible as a consequence of the uniqueness shown in Theorem 4.15. If this uniqueness did not hold, a pessimistic approach would have to be taken, in which the leader chooses flows and potentials most in favor of the TSO, thus resulting in a trilevel problem. In Problem (4.7), the nonlinear constraint (3.4b) is at the upper level, and so are the flows q and potentials π. In particular, the indicator functions χ_a can be modeled by introducing a new binary variable s_a for each $a \in A_{\text{act}}$ together with Constraints (4.7e) at the upper level. While the new upper level is a nonconvex MINLP, the TSO's problem is now an LP for a fixed upper-level decision (ℓ, q, π, s). Consequently, the single-level reformulations presented in Section 2.2 can be applied to Problem (4.7). Section 5 of [FP5] presents the KKT reformulation of (4.7). Therein, provably correct big-Ms are also derived to be used in a linearization of the KKT complementarity conditions.

In the remainder of this section, we present three explicit formulas of the optimal value function of the lower level. These yield three optimal-value-function reformulations of Problem (4.7) and lead to novel characterizations of feasible bookings on active networks satisfying Assumption 4.14.

Problem (4.7) is a max-min bilevel problem, which also include interdiction-like problems; see Smith and Song (2020) for a recent survey. Leader and follower share the same objective function, but with different optimization directions. Note also that for every leader decision, the TSO may set the controls Δ and shifts τ to zero and adapt the violations y and z to match the leader's potential-based flow. Consequently, the lower level is always feasible. The optimal-value-function reformulation of (4.7) is therefore given by

$$\max_{\ell,q,\pi,s} \{\varphi(\ell,q,\pi,s)\colon \text{(4.7b)–(4.7f)}\}\,. \tag{4.9}$$

In contrast to the presentation of optimal-value-function reformulations of Section 2.2, the max-min structure allows us to directly set the follower's optimal value function φ as the leader's objective function. Furthermore, since the feasibility of the lower level is always guaranteed, the lower-level constraints are omitted such that the feasible domain of (4.9) is only determined by upper-level feasibility.

The optimal value function φ of the lower level (4.8) is equivalently defined by its dual problem, since strong duality holds. To present the dual of the lower level for a fixed upper-level decision (ℓ,q,π,s), we introduce dual variables α_a for $a \in A_{\text{act}}$ for Constraints (4.8b), δ_u^- and δ_u^+ for $u \in V$ corresponding to (4.8d) and (4.8e), and finally β_a for $a \in A_{\text{act}}$ associated to the upper bound on Δ_a. The dual of Problem (4.8) is then given by

$$\begin{aligned}
\max_{\alpha,\beta,\delta^+,\delta^-} \quad & -\sum_{a\in A_{\text{act}}} \Delta_a^+ s_a \beta_a + \sum_{u\in V} \left((\pi_u^- - \pi_u)\delta_u^- - (\pi_u^+ - \pi_u)\delta_u^+\right) && \text{(4.10a)}\\
\text{s.t.} \quad & \sum_{a\in\delta^{\text{out}}(G_j)} \alpha_a - \sum_{a\in\delta^{\text{in}}(G_j)} \alpha_a = \sum_{u\in V(G_j)} (\delta_u^+ - \delta_u^-), \quad G_j \in \mathcal{G}, && \text{(4.10b)}\\
& \alpha_a \le \beta_a,\ \beta_a \ge 0, \quad a \in A_{\text{cm}}, && \text{(4.10c)}\\
& -\alpha_a \le \beta_a,\ \beta_a \ge 0, \quad a \in A_{\text{cv}}, && \text{(4.10d)}\\
& \sum_{u\in V} \delta_u^+ = 1,\ \sum_{u\in V} \delta_u^- = 1, && \text{(4.10e)}\\
& \delta_u^+, \delta_u^- \ge 0, \quad u \in V. && \text{(4.10f)}
\end{aligned}$$

For a given upper-level decision (ℓ,q,π,s), the optimal value $\varphi(\ell,q,\pi,s)$ is attained at a vertex of the feasible polyhedron of the lower level's dual problem. Consequently, φ is given by the maximum of linear functions, evaluated in vertices of (4.10b)–(4.10f), and thus a piecewise-linear and convex function. As a result, solving the optimal-value-function reformulation (4.9) consists in maximizing a convex function over a nonconvex feasible set. Expressing the optimal value function in terms of all vertices of the lower level's dual problem is difficult in general, since there can be a possibly exponential number of vertices. In [FP5], we show that there exists a polynomial number of vertices of (4.10) that can be explicitly computed. Furthermore, they can be directly linked to the structure of the network. Let $A_{\mathrm{cm}}^{j,\rightarrow}$ and $A_{\mathrm{cm}}^{j,\leftarrow}$ be the sets of compressors $a \in A_{\mathrm{cm}}$ that are directed towards or away from a passive subnetwork $G_j \in \mathcal{G}$. Under Assumption 4.14, these sets are well defined and $A_{\mathrm{cv}}^{j,\rightarrow}$ and $A_{\mathrm{cv}}^{j,\leftarrow}$ are defined similarly for control valves $a \in A_{\mathrm{cv}}$. This allows us to present the first closed-form formula of the lower-level optimal value function.

Theorem 4.17 (Corollary 6.3 in [FP5]). *The optimal value $\varphi(\ell, q, \pi, s)$ of (4.8) is given by*

$$\max_{\substack{(G_{j_1}, G_{j_2}) \in \mathcal{G}^2,\\ w_1 \in V(G_{j_1}),\\ w_2 \in V(G_{j_2})}} \left\{ \pi_{w_1} - \pi_{w_2} - \left(\pi_{w_1}^+ - \pi_{w_2}^- + \sum_{\substack{a \in P(G_{j_1}, G_{j_2}):\\ a \in A_{\mathrm{cm}}^{j_1,\rightarrow} \cup A_{\mathrm{cv}}^{j_1,\leftarrow}}} \Delta_a^+ s_a \right) \right\}. \tag{4.11}$$

As previously discussed, (4.11) is a piecewise-linear and convex function. Substituting the optimal value function in (4.9) yields a max-max problem. It is then possible to exchange the maximization over (ℓ, q, π, s) satisfying (4.7b)–(4.7f) and the discrete max-operator over all pairs of nodes $(w_1, w_2) \in V^2$. This results in the following characterization of feasible bookings.

Corollary 4.18 (Theorem 6.4 in [FP5]). *Let $G = (V, A)$ be a weakly connected network satisfying Assumption 4.14. 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*

$$\phi_{w_1 w_2}(b) := \max_{\ell, q, \pi} \left\{ \pi_{w_1} - \pi_{w_2} - \sum_{\substack{a \in P(G_{j_1}, G_{j_2}):\\ a \in A_{\mathrm{cm}}^{j_1,\rightarrow} \cup A_{\mathrm{cv}}^{j_1,\leftarrow}}} \Delta_a^+ s_a \colon \text{(4.7b)–(4.7f)} \right\}. \tag{4.12}$$

This characterization of feasible bookings on active networks with the structure given by Assumption 4.14 generalizes the characterization of Theorem 4.2. Indeed, if a passive network is considered, i.e., $A_{\mathrm{act}} = A_{\mathrm{cm}} \cup A_{\mathrm{cv}} = \emptyset$, then Problem (4.12) is equivalent to (4.3). In the active case, the characterization still requires the computation of nominations with maximum potential difference between a pair of nodes $(w_1, w_2) \in V^2$. However, now, it is taken into account that the TSO reacts optimally by choosing an appropriate control of the active elements countering the potential drop. The active elements influencing the potential difference between w_1 and w_2 lie on the path $P(G_{j_1}, G_{j_2})$. Making use of elements in $A_{\mathrm{cm}}^{j_1,\leftarrow} \cup A_{\mathrm{cv}}^{j_1,\rightarrow}$ would result in an even larger potential difference between w_1 and w_2. These elements are thus set to zero. On the other hand, elements in $A_{\mathrm{cm}}^{j_1,\rightarrow} \cup A_{\mathrm{cv}}^{j_1,\leftarrow}$ allow to reduce the potential difference, and are used at their maximum capacity from the point of view of the TSO, i.e., $\Delta_a = \Delta_a^+ s_a$ for all $a \in A_{\mathrm{cm}}^{j_1,\rightarrow} \cup A_{\mathrm{cv}}^{j_1,\leftarrow}$.

Whenever the TSO uses the active elements, their settings influence all node potentials of a passive subnetwork. Instead of considering all nodes individually, they can be grouped w.r.t. the passive subnetworks they belong to. We apply this transformation to the lower-level optimal value function.

Theorem 4.19. *The optimal value $\varphi(\ell, q, \pi, s)$ of (4.8) is given by*

$$\max_{(G_{j_1}, G_{j_2}) \in \mathcal{G}^2} \left\{ \theta^+_{j_1} + \theta^-_{j_2} - \sum_{\substack{a \in P(G_{j_1}, G_{j_2}): \\ a \in A^{j_1, \rightarrow}_{\mathrm{cm}} \cup A^{j_1, \leftarrow}_{\mathrm{cv}}}} \Delta^+_a s_a \right\}, \tag{4.13}$$

where for every $G_j \in \mathcal{G}$, we define

$$\begin{aligned} \theta^+_j &:= \max_{u \in V(G_j)} \left\{ \pi_u - \pi^+_u \right\}, \\ \theta^-_j &:= \max_{u \in V(G_j)} \left\{ \pi^-_u - \pi_u \right\}. \end{aligned}$$

The inner max-operators determine the maximum violation of upper and lower potential bounds within each passive subnetwork. This closed-form formula of the optimal value function reflects that the TSO's optimal reaction is the same for all pairs of nodes $w_1 \in V(G_{j_1})$ and $w_2 \in V(G_{j_2})$. It is then again possible to derive a characterization.

Corollary 4.20 (Corollary 6.5 in [FP5])**.** *Let $G = (V, A)$ be a weakly connected network satisfying Assumption 4.14. Then, the booking $b \in L$ is feasible if and only if $\phi_{j_1 j_2}(b) \le 0$ is satisfied for every pair of passive subnetworks $(G_{j_1}, G_{j_2}) \in \mathcal{G}^2$, where we define*

$$\begin{aligned} \phi_{j_1 j_2}(b) := \max_{\ell, q, \pi} \quad & \theta^+_{j_1} + \theta^-_{j_2} - \sum_{\substack{a \in P(G_{j_1}, G_{j_2}): \\ a \in A^{j_1, \rightarrow}_{\mathrm{cm}} \cup A^{j_1, \leftarrow}_{\mathrm{cv}}}} \Delta^+_a s_a && \text{(4.14a)} \\ \text{s.t.} \quad & \text{(4.7b)–(4.7f)}, \\ & \theta^+_{j_1} = \max_{u \in V(G_{j_1})} \left\{ \pi_u - \pi^+_u \right\}, && \text{(4.14b)} \\ & \theta^-_{j_2} = \max_{u \in V(G_{j_2})} \left\{ \pi^-_u - \pi_u \right\}. && \text{(4.14c)} \end{aligned}$$

The number of subproblems to be solved in Corollary 4.20 is reduced to $|\mathcal{G}|^2 = (|A_{\mathrm{act}}| + 1)^2$ compared to $|V|^2$ many subproblems in Corollary 4.18. This reduction comes at the cost of more challenging optimization problems. While the objective function of (4.12) is linear, we now maximize the sum of two piecewise-linear functions in each subproblem (4.14).

For networks with many active elements, the number of subproblems quadratic in the number of passive components might still be a computational drawback. To derive a characterization with a number of subproblems that is linear in the number of passive subnetworks, we consider a third representation of the lower-level optimal value function. Given the tree structure of the reduced network $\tilde{G}$ under

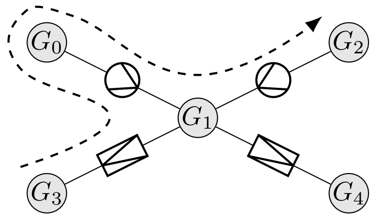

Figure 4.6: Example for which the inequality in (4.16) is strict (taken from [FP5]).

Assumption 4.14, it is possible to extend arguments from Section 4.2 to the active case. Therein, the maximum potential difference $\pi_{w_1} - \pi_{w_2}$ is determined in a separable way after splitting it w.r.t. an arbitrary reference node o. The optimal solution is computed by maximizing $\pi_{w_1} - \pi_o$ and $\pi_o - \pi_{w_2}$. In the active case, we can apply a similar reasoning. Considering an intermediate passive subnetwork $G_k \in \mathcal{G}$ allows us to separate the contribution of the active elements along the paths $P(G_k, G_{j_1})$ and $P(G_k, G_{j_2})$. This leads to the third representation of the lower-level optimal value function φ.

Theorem 4.21 (Theorem 6.7 in [FP5]). *The optimal value $\varphi(\ell, q, \pi, s)$ of (4.8) is given by*

$$\max_{G_k \in \mathcal{G}} \left\{ \vartheta_k^+ + \vartheta_k^- \right\}, \tag{4.15}$$

where for every $G_k \in \mathcal{G}$, we define

$$\vartheta_k^+ := \max_{\substack{G_j \in \mathcal{G},\\ u \in V(G_j)}} \left\{ \pi_u - \pi_u^+ - \sum_{\substack{a \in P(G_k, G_j):\\ a \in A_{\mathrm{cm}}^{k,\leftarrow} \cup A_{\mathrm{cv}}^{k,\rightarrow}}} \Delta_a^+ s_a \right\},$$

$$\vartheta_k^- := \max_{\substack{G_j \in \mathcal{G},\\ u \in V(G_j)}} \left\{ \pi_u^- - \pi_u - \sum_{\substack{a \in P(G_k, G_j):\\ a \in A_{\mathrm{cm}}^{k,\rightarrow} \cup A_{\mathrm{cv}}^{k,\leftarrow}}} \Delta_a^+ s_a \right\}.$$

The intuition is that for a triplet of passive subnetworks $(G_{j_1}, G_k, G_{j_2}) \in \mathcal{G}^3$,

$$\sum_{\substack{a \in P(G_{j_1}, G_{j_2}):\\ a \in A_{\mathrm{cm}}^{j_1,\rightarrow} \cup A_{\mathrm{cv}}^{j_1,\leftarrow}}} \Delta_a^+ s_a \leq \sum_{\substack{a \in P(G_k, G_{j_1}):\\ a \in A_{\mathrm{cm}}^{k,\leftarrow} \cup A_{\mathrm{cv}}^{k,\rightarrow}}} \Delta_a^+ s_a + \sum_{\substack{a \in P(G_k, G_{j_2}):\\ a \in A_{\mathrm{cm}}^{k,\rightarrow} \cup A_{\mathrm{cv}}^{k,\leftarrow}}} \Delta_a^+ s_a \tag{4.16}$$

is satisfied and equality holds if G_k lies on the path $P(G_{j_1}, G_{j_2})$. Figure 4.6 illustrates this relation for $G_{j_1} = G_3$, $G_k = G_0$, and $G_{j_2} = G_2$. Here, the active arc (G_0, G_1) is accounted for in the sum at the right-hand side of (4.16), while clearly not lying on $P(G_{j_1}, G_{j_2})$ and thus not appearing at the left-hand side. However, if one considers $G_k = G_1$ equality holds. By first maximizing over G_k, the selection of G_{j_1} and G_{j_2} becomes separable. Then, ϑ_k^+ determines G_{j_1} such that the potential differences between nodes of G_{j_1} and G_k are maximal. Similarly, ϑ_k^- determines G_{j_2}. The characterization corresponding to this variant of the optimal value function is given by the following corollary.

Corollary 4.22 (Corollary 6.8 in [FP5]). *Let $G = (V, A)$ be a weakly connected network satisfying Assumption 4.14. Then, the booking $b \in L$ is feasible if and only if $\phi_k(b) \le 0$ is satisfied for every passive subnetwork $G_k \in \mathcal{G}$, where we define*

$$\begin{aligned}
\phi_k(b) := \max_{\ell,q,\pi} \quad & \vartheta_k^+ + \vartheta_k^- \\
\text{s.t.} \quad & \text{(4.7b)–(4.7f)}, \\
& \vartheta_k^+ = \max_{\substack{G_j \in \mathcal{G},\\ u \in V(G_j)}} \left\{ \pi_u - \pi_u^+ - \sum_{\substack{a \in P(G_k, G_j):\\ a \in A_{\text{cm}}^{k,\leftarrow} \cup A_{\text{cv}}^{k,\rightarrow}}} \Delta_a^+ s_a \right\}, \\
& \vartheta_k^- = \max_{\substack{G_j \in \mathcal{G},\\ u \in V(G_j)}} \left\{ \pi_u^- - \pi_u - \sum_{\substack{a \in P(G_k, G_j):\\ a \in A_{\text{cm}}^{k,\rightarrow} \cup A_{\text{cv}}^{k,\leftarrow}}} \Delta_a^+ s_a \right\}.
\end{aligned}$$

The number of subproblems is thus successfully reduced to $|\mathcal{G}| = |A_{\text{act}}| + 1$, at the cost of more complex inner piecewise-linear functions. For a passive subnetwork $G_k \in \mathcal{G}$, the piecewise-linear functions θ_k^+ and θ_k^- each consist of $|V(G_k)|$ pieces, whereas ϑ_k^+ and ϑ_k^- both have $|V|$ many.

The three optimal-value-function reformulations and the resulting characterizations provide us with a variety of methods to check the feasibility of bookings. Model sizes and number of optimization problems to be solved thereby strongly depend on the structure of the network. In the next section, we compare our methods in a case study of two networks with different compositions.

4.5 Computational Study

In [FP5], we evaluate the performance of our various approaches to determine the feasibility of a booking in a case study of two networks from the GasLib (Schmidt et al. 2017). On the one hand, we study the GasLib-134 network, which has 134 nodes, one compressor, one control valve, and no cycles, i.e., it is a tree. On the other hand, we study a modified version of the GasLib-40 network, in which we replace one compressor by a pipe to satisfy Assumption 4.14. The resulting network has 40 nodes, five compressors, and six fundamental cycles, which are the cycles generated by adding an arc to a spanning tree. The respective bookings are obtained by setting a nomination from the GasLib as a booking. As a benchmark, we compare our methods to the KKT reformulation of Problem (4.7) with linearized complementarity constraints. Similarly, all piecewise-linear functions in the three optimal-value-function reformulations or the subproblems of the three characterizations are linearized by

Table 4.1: Overview of methods and model statistics (taken from [FP5]).

Method	Definition	GasLib-134 Subproblems	GasLib-134 Binaries	GasLib-40 Subproblems	GasLib-40 Binaries
KKT		1	272	1	90
F-OVF	(4.9) using (4.11)	1	17956	1	1600
R-OVF	(4.9) using (4.13)	1	277	1	116
S-OVF	(4.9) using (4.15)	1	807	1	486
F-CHAR	Corollary 4.18	17956	0	1600	0
R-CHAR	Corollary 4.20	9	162	36	44
S-CHAR	Corollary 4.22	3	268	6	80

introducing one additional binary variable per piece. In addition to the problem-specific variables, all approaches thus require additional binary variables. Their number varies greatly with the considered approach as well as the network structure and, more precisely, the numbers of nodes $|V|$ and of active elements $|A_{\text{act}}|$. The number of subproblems to be solved in a characterization is equal to the number of pieces in the representation of the lower-level optimal value function. It thus also depends on $|V|$ and $|A_{\text{act}}|$. Table 4.1 summarizes the methods studied and presents some model statistics w.r.t. GasLib-134 and GasLib-40. The columns Subproblems and Binaries indicate the number of subproblems to be solved and the maximum number of additional binary variables necessary for the linearization of each subproblem. Single-level reformulations KKT, F-OVF, R-OVF, and S-OVF consist in the resolution of a single MINLP, whereas the characterizations F-CHAR, R-CHAR, and S-CHAR require several MINLP subproblems to be solved.

Our computational experiments have shown that the nonlinear gas physics modeled by Constraints (3.4b) result in significant challenges for state-of-the-art MINLP solvers. We therefore focus our presentation on the linear approximations studied in [FP5]. 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, Constraints (3.4b) are replaced with

$$\pi_u - \pi_v = \xi_a q_a, \quad \xi_a = c\Lambda_a M, \quad a = (u,v) \in A_{\text{pipe}}.$$

In [FP5], we consider multiple scaling factors c. However, since the trends observed are comparable for all choices of the scaling factor, we summarize the main findings for $c = 0.2$. The booking considered on GasLib-134 is derived from the 2011-11-06 nomination of the GasLib. For GasLib-40, we use the booking derived from the single corresponding nomination of the GasLib. For a full overview of the computational setup and in-depth analyses of the nonlinear and linear cases, we refer the reader to Section 7 of [FP5].

Table 4.2 shows the results for the GasLib-134 network and the 2011-11-06 booking. The column Vio. measures the violation corresponding to the booking, i.e., the

Table 4.2: Results for GasLib-134 (taken from [FP5]).

		Time		
Method	Vio.	Sol.	Max.	Total
KKT	-377.15	2.71		2.75
R-OVF	-377.15	2.02		2.06
S-OVF	-377.15	4.53		4.62
R-CHAR	-377.15		0.65	2.87
S-CHAR	-377.15		1.14	3.00

optimal value of single-level reformulations and the maximum violation of any bound on the optimal solutions of the characterization subproblems. A positive violation indicates that there is a booking-compliant nomination that violates the potential bounds. In that case the booking is infeasible. For nonpositive values, all booking-compliant nominations can be transported without violation and the booking is thus feasible. The column Sol. measures the time necessary to solve a single-level reformulation in seconds, whereas Total also accounts for the model creation. For characterizations, Max. indicates the maximum amount of time (in seconds) spent in solving one subproblem. Note that all subproblems can be solved independently and in parallel. For a fully parallelized algorithm based on the characterizations, Max. therefore represents an idealized parallel time. In this case, Total (in seconds) measures the model creation time and the total sequential time necessary to solve all subproblems. Due to their large numbers of subproblems or binary variables, F-OVF and F-CHAR are significantly outperformed by the other methods and are therefore dropped from the table. Observe that the 2011-11-06 booking is feasible for the scaling factor $c = 0.2$. All methods listed in the table perform at the same order of magnitude. On GasLib-134, R-OVF is the fastest single-level reformulation of Problem (4.7), which slightly outperforms KKT and runs more than twice as fast as S-OVF. In terms of total sequential time, R-OVF also outperforms R-CHAR and S-CHAR, which are based on the characterizations. However, in terms of idealized parallel time, R-CHAR is the overall fastest method. It requires the resolution of nine subproblems with at most 162 additional binary variables for the linearization of piecewise-linear functions. In comparison, only three subproblems need to be solved for S-CHAR, but up to 268 additional binary variables are required. Although, both R-CHAR and S-CHAR admit comparable sequential times, we can observe the trade-off between the smaller number of subproblems and the larger time spent on branching on the additional binary variables.

The results corresponding to GasLib-40 are presented in Table 4.3. Since the network has fewer nodes than GasLib-134, F-OVF and F-CHAR are now more tractable and thus shown in the table. On the other hand, the cyclic structure and higher number of active elements of GasLib-40 make checking the feasibility of the booking more challenging for all methods. S-OVF is not able to find a provably optimal solution within the time limit of two hours for our experiments and has been omitted

Table 4.3: Results for GasLib-40 (taken from [FP5]).

Method	Vio.	Time		
		Sol.	Max.	Total
KKT	1792.45	2.79		2.83
F-OVF	1792.45	15.24		15.45
R-OVF	1792.45	7.38		7.43
F-CHAR	1792.45		0.47	197.37
R-CHAR	1792.45		0.44	5.23
S-CHAR	1792.45		2.06	11.44

from the table. The booking is infeasible since Vio. is positive for all methods. In terms of total time, KKT is the fastest method to come to this conclusion. It is only outperformed by all three approaches based on the characterizations if we consider the idealized parallel time. Here, F-CHAR and R-CHAR both perform in under 0.5 s and thus outperform S-CHAR by a factor of four. It should however be noted that in order to achieve this performance for F-OVF, 1600 subproblems need to be solved in parallel, which seems unrealistic. If there is a sufficient number of cores to fully parallelize the 36 subproblems, R-CHAR is the best-performing method. Otherwise, if parallel computing resources are more restricted, S-CHAR presents a valuable alternative with only six subproblems to be solved in parallel.

Overall, the various methods presented in Section 4.4 and compared in this section provide a great flexibility, when checking the feasibility of a booking. While methods based on the single-level reformulations tackle the task by solving a single, larger optimization problem, solving the subproblems of the characterizations can be fully parallelized. The "best" method then depends on the availability of parallel computing resources as well as the network structure. While one approach might perform better on networks with many nodes and few active elements, another method might be a better choice for networks with many active elements but only few nodes per passive subnetwork. In practice, the generic KKT-based approach is already a good choice. Usually, a TSO has additional insights on bottlenecks of the network and a thorough knowledge based on historic events. In that perspective, the characterizations are useful to only check specific subproblems and very quickly detect infeasibility. More generally, all methods presented can in practice be terminated early, as soon as an infeasible nomination is detected.

5

Conclusion

Gas networks are an important infrastructure for the overall energy supply in Europe—now and in the future. After the liberalization of the European gas markets, the access to these networks is guaranteed via booking contracts and subsequent nominations. In this dissertation, we have studied the feasibility of bookings, one of the central capacity-right contracts in the European entry-exit market system. A variety of results have been derived. On the one hand, we studied general passive networks and considered in depth the special cases of trees and single cycles. On the other hand, we considered networks with linearly modeled active elements. The latter case naturally led us to consider bilevel formulations to model the feasibility of a booking.

In a first phase, our more general study of linear bilevel problems has therefore been presented. In [FP1], it is shown that validating bilevel-correct big-Ms is hard if problem-specific knowledge cannot be used. In general, the validation task is as hard as solving the original bilevel problem. While we only considered LP-LP bilevel problems, the hardness results of validating big-Ms directly carry over to more general classes of bilevel problems for which the KKT reformulation can be applied. However, in some cases, problem-specific knowledge is indeed missing and bilevel-correct big-Ms cannot be easily determined. The KKT reformulation can still be used to solve a linear bilevel problem by branching on the complementarity constraints via the SOS1 capabilities of state-of-the-art mixed-integer solvers. In [FP2], we derive a new family of valid inequalities from the strong-duality constraint of the linear lower level. Our experiments suggest that they decrease resolution times by reintroducing the coupling of primal and dual variables of the lower level, that is missing in the root relaxation of an SOS1-based branch-and-bound algorithm. In accordance with the studies by Pineda et al. (2018) and Kleinert and Schmidt (2020a), one can therefore conclude that an SOS1-based branch-and-cut algorithm equipped with our valid inequality provides a promising big-M-free alternative to solve linear bilevel problems.

After the presentation of the more general results on linear bilevel problems, we have then focused on feasible bookings in the European entry-exit gas market.

We started by presenting our results for passive networks, for which single-level approaches are sufficient. In [FP3], the feasibility of a booking on passive networks is characterized by a finite and polynomial number of nominations. The latter are solutions of nonlinear and nonconvex optimization problems, which maximize the potential difference between every pair of nodes in the network. The booking is feasible if and only if these maximum potential differences satisfy given bounds. While Thürauf (2020) shows that deciding the feasibility of a booking on passive networks is coNP-hard in general, we prove that the maximum potential differences between every pair of nodes can be computed efficiently on passive trees. Consequently, the feasibility of a booking can be decided in polynomial time in this case. Furthermore, the in-depth structural analysis in [FP4] of nominations that lead to maximum potential differences allows us to conclude that the same holds for single passive cycles. Together with the studies by Hayn (2017), Robinius et al. (2019), Schewe et al. (2020a,c), and Thürauf (2020), our work provides an extensive overview of the computational complexity of deciding the feasibility of a booking on passive networks as well as important structural insights.

In contrast to passive networks, where most variables are fixed by physics once a nomination is given, the TSO actively influences gas flows in active networks. In [FP5], a first stepping stone is laid for the study of feasible bookings on active networks. We derive a bilevel model to check the feasibility of a booking on networks with linearly modeled active elements and taking into account that the TSO reacts optimally to every nomination. This bilevel problem with a nonlinear and nonconvex lower level mirrors the highly challenging nature of deciding the feasibility of a booking. Under the assumption that no active element lies on an undirected cycle in the network, we recast the bilevel problem into an equivalent model, where the upper level is now an MINLP and the lower level is an LP. On the one hand, by exploiting the structure of the TSO's problem at the lower level and its dual, we obtain provably correct big-Ms for the KKT reformulation with linearized complementarity constraints. The specific structure of the bilevel model thus allows us to circumvent the difficulties of validating big-Ms as discussed in [FP1]. On the other hand, we extract a polynomial number of vertices of the dual feasible region of the lower level that allow to fully describe the lower-level optimal value function—a task that is very difficult in general. Various reformulations of the lower-level optimal value function are discussed, which lead to novel characterizations of feasible bookings on active networks. The combination of bilevel techniques and the specific insights on gas flows thus gives rise to a wide range of new approaches to check the feasibility of a booking.

Overall, we have made significant contributions in linear bilevel optimization and in the study of feasible bookings in the European entry-exit gas market. Nonetheless, there remain important open questions and challenges. The two proxies discussed in [FP1] for bilevel-correct big-Ms in bilevel optimization are only sufficient conditions and disregard the optimality of the upper level. It thus remains to find necessary and sufficient conditions that characterize bilevel-correct big-Ms and take into account the optimality of the original bilevel problem. Such a characterization would allow to determine the smallest bilevel-correct big-Ms, which could in turn greatly benefit the resolution of bilevel problems via their KKT reformulation with linearized complementarity constraints. In theory, it is therefore highly interesting to determine necessary and sufficient conditions for bilevel-correct big-Ms. However, as a consequence of the already observed hardness results in [FP1], it is very likely that validating or computing big-Ms w.r.t. this characterization would result in an even harder task than for the discussed proxies.

One of the major challenges when developing and testing approaches for general LP-LP bilevel optimization, such as the big-M-free branch-and-cut algorithm presented in [FP2], is the availability of diverse bilevel instances. Our test set has been generated by taking mixed-integer linear bilevel instances from the literature and relaxing the integrality constraints. In many cases, this results in continuous bilevel instances that are too easy, since the difficulty of the original instance might exactly arise from the integrality constraints. Furthermore, a lot of the original instances considered in the computational study of [FP2] are taken from the literature on interdiction-like problems and have therefore a very specific structure. It would be beneficial to test the valid inequalities in [FP2] on a more diverse test set and determine problem characteristics which promote their utility. It is possible to extend the rationale of [FP2] to a broader class of bilevel problems, as long as strong duality holds at the lower level. This would then allow to integrate more instances from the literature into the test set. Nonetheless, the valid inequalities can be easily implemented and used at the root node of various problems in the field of LP-LP bilevel optimization; see, e.g., Besançon et al. (2019).

As for deciding the feasibility of bookings, many new computational complexity results have been derived over the last years and in this dissertation. However, the most general class of networks for which the problem can be decided in polynomial time still needs to be determined if nonlinear potential-based flows are used. The passive network used in the proof of coNP-hardness by Thürauf (2020) most notably contains cycles with shared edges. One could thus investigate the case of passive networks with edge-disjoint cycles, so-called cactus graphs. It might then be possible to derive new insights by combining the results of [FP3] on passive trees and [FP4] on single passive cycles. Furthermore, it is also not clear if the problem is in coNP if nonlinear potential-based flows are used, since it is still unknown if a certificate of infeasibility of polynomial size exists. The issue with the certificate presented in [FP3] was the use of the flows corresponding to a nomination. This in particular requires taking roots, which may result in irrational flows. Based on the characterization of feasible bookings derived in [FP3] and if flow bounds are neglected, it might be possible to obtain a valid certificate in terms of potential differences. However, deriving a valid certificate becomes more difficult if explicit flow bounds need to be considered.

On the more practical side, most gas networks contain active elements to counter the potential loss caused in the pipes. In [FP5], we consider compressors and control valves for which the action on the potentials is linear and additive. When considering more detailed models for the active elements, this action is usually multiplicative and thus nonlinear; see, e.g., Borraz-Sánchez et al. (2016). The initial bilevel model of [FP5] can be extended to take these more general active elements into account. However, the KKT conditions are then no longer necessary and sufficient for the optimality of the lower level and different reformulations, e.g., based on the lower-level optimal value function, must be used. Even using linear models for the active elements, our techniques strongly depend on the assumption that active elements do not lie on undirected cycles in the network. If this assumption is dropped in an effort to model more realistic networks, the uniqueness of flows is no longer guaranteed. As a consequence, the nonlinear gas physics can no longer be moved from the TSO's problem at the lower level to the upper level and alternative (re)formulations and algorithms are required. If the assumption holds, our computational experiments have shown that nonlinear gas physics remain challenging, which illustrates the necessity for problem-tailored solution approaches. Here, many of the techniques that have been successfully applied for nominations could be studied and extended w.r.t. bookings. In our experiments, the KKT reformulation with linearized complementarity constraints performs well, but larger networks might lead to weak relaxations due to the choice of big-Ms. In this case, a big-M-free approach like the branch-and-cut proposed in [FP2] could be considered.

Finally, the feasibility of bookings is only one puzzle piece in the bigger picture of the European entry-exit gas market. In line with the studies by Grimm et al. (2019), Böttger et al. (2020), Schewe et al. (2020b), and Heitsch et al. (2021), the author of this dissertation believes that the variety of theoretical results and solution approaches presented in this work can be helpful in future studies of this market system.

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Part II

Reprints of Published Journal Articles and Preprints

Article 1

Technical Note—There's No Free Lunch: On the Hardness of Choosing a Correct Big-M in Bilevel Optimization

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There's No Free Lunch: On the Hardness of Choosing a Correct Big-M in Bilevel Optimization

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Abstract. One of the most frequently used approaches to solve linear bilevel optimization problems consists in replacing the lower-level problem with its Karush–Kuhn–Tucker (KKT) conditions and by reformulating the KKT complementarity conditions using techniques from mixed-integer linear optimization. The latter step requires to determine some big-M constant in order to bound the lower level's dual feasible set such that no bilevel-optimal solution is cut off. In practice, heuristics are often used to find a big-M although it is known that these approaches may fail. In this paper, we consider the hardness of two proxies for the above mentioned concept of a bilevel-correct big-M. First, we prove that verifying that a given big-M does not cut off any feasible vertex of the lower level's dual polyhedron cannot be done in polynomial time unless $\mathsf{P} = \mathsf{NP}$. Second, we show that verifying that a given big-M does not cut off any optimal point of the lower level's dual problem (for any point in the projection of the high-point relaxation onto the leader's decision space) is as hard as solving the original bilevel problem.

1. Introduction

A bilevel optimization problem consists in a constrained optimization problem in which some constraints specify that a subset of variables constitutes an optimal solution of a second (auxiliary) optimization problem. Since the publication of the first and seminal paper [7], research on the subject has become increasingly important. Indeed, the bilevel structure allows the modeling of a large number of real-life problems involving two types of decision makers, a leader and a follower (or several followers) interacting hierarchically. Such optimization problems appear in many fields of application like energy markets [1, 10, 18–21, 23, 25], critical infrastructure defense [8, 9, 14, 29], or pricing [26, 27, 31].

Due to their ability of modeling hierarchical decision processes, bilevel optimization problems are inherently hard to solve. In [13, 22] it is shown that even the easiest instantiation, i.e., bilevel problems with linear upper and lower level, is strongly NP-hard. Moreover, even checking local optimality for a given point is NP-hard as well [32]. For other hardness results we refer to, e.g., [5]. For general surveys of bilevel optimization see [4, 11–13] and [33] for a survey focusing on linear-linear (LP-LP) bilevel problems.

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In this paper, we consider the LP-LP bilevel problem

$$\min_{x\in\mathbb{R}^n, y\in\mathbb{R}^m} \quad c^\top x + d^\top y \tag{1a}$$

$$\text{s.t.} \quad Ax + By \geq a, \tag{1b}$$

$$y \in \arg\min_{\bar{y}} \{f^\top \bar{y} \colon Cx + D\bar{y} \geq b\} \tag{1c}$$

with $c \in \mathbb{R}^n$, $d, f \in \mathbb{R}^m$, $A \in \mathbb{R}^{k\times n}$, $B \in \mathbb{R}^{k\times m}$, $a \in \mathbb{R}^k$, $C \in \mathbb{R}^{\ell\times n}$, $D \in \mathbb{R}^{\ell\times m}$, and $b \in \mathbb{R}^\ell$. Problem (1a)–(1b) is the so-called upper level and (1c) is the lower level. Here, we consider the optimistic version of bilevel optimization [12]. This means that whenever the lower-level problem has multiple solutions y, the leader chooses the most favorable one in terms of the upper level's problem.

LP-LP bilevel problems are often solved by a reformulation to an equivalent single-level problem. Usually, this is done by one of the following two approaches. One can replace the lower level with its primal and dual feasibility conditions as well as the strong-duality equation or one replaces the lower level with its Karush–Kuhn–Tucker (KKT) conditions. Both approaches have their drawbacks: The strong-duality based technique yields nonconvex bilinear terms whereas the KKT approach leads to the following mathematical program with complementarity constraints (MPCC):

$$\min_{x,y,\lambda} \quad c^\top x + d^\top y \tag{2a}$$

$$\text{s.t.} \quad Ax + By \geq a, \ D^\top \lambda = f, \tag{2b}$$

$$0 \leq Cx + Dy - b \perp \lambda \geq 0. \tag{2c}$$

Here, for two non-negative vectors $0 \leq a, b \in \mathbb{R}^n$, $a \perp b$ abbreviates $a_i b_i = 0$ for all $i = 1, \ldots, n$. The single-level reformulation (2) of the bilevel problem (1) explicitly models the optimistic version of bilevel optimization by construction. Consequently, there is no need anymore to distinguish between y and $\bar{y}$. In what follows, we thus call x the upper-level and y the lower-level (primal) variables. The lower-level dual variables are given by $\lambda \in \mathbb{R}^\ell$.

The hardness of Problem (2) stems from the complementarity conditions (2c). Since these constraints can be reformulated in a mixed-integer linear way, the KKT approach is often preferred in practice. Typically, one applies the reformulation introduced in [15], which requires an additional binary variable $z_i \in \{0, 1\}$ for every $i \in \{1, \ldots, \ell\}$ and the additional constraints

$$\lambda_i \leq M_{\mathrm{d}} z_i, \quad (Cx + Dy - b)_i \leq (1 - z_i) M_{\mathrm{p}}, \quad i \in \{1, \ldots, \ell\}, \tag{3}$$

where M_{d} and M_{p} are sufficiently large constants, called big-Ms. In this note, we focus on the big-M for bounding the lower-level dual variables, i.e., on $M = M_{\mathrm{d}}$. Since we show that finding M_{d} is hard, this obviously implies that finding M_{d} and M_{p} is hard as well. Applying (3) requires to bound the lower level's dual polyhedron such that no point λ^* that is part of an optimal solution (x^*, y^*, λ^*) of (2) is cut off. Stated differently, one needs to choose an M that preserves all bilevel-optimal points (x^*, y^*). We call an M with this property a *bilevel-correct* big-M.

When the dual of the lower level has a finite optimal value, there exists an optimal solution λ^* that is a vertex of the associated feasible polyhedron. Hence, it is sufficient to obtain bounds on the dual variables that—independently of the upper-level decision—do not cut off (i) any feasible vertex of the lower level's dual polyhedron or (ii) any optimal vertex of the lower level's dual polyhedron. Note that these requirements do not take into account bilevel optimality but still preserve all optimal solutions (x^*, y^*, λ^*) of (2), i.e., (i) and (ii) still yield bilevel-correct big-M's. This means, that (i) and (ii) are sufficient (but not necessary) conditions for a big-M to be bilevel-correct.

The choice of the big-M is often done heuristically, which may result in a severe issue: If the big-M is not chosen large enough, a "solution" of (2) with (2c) replaced by (3) does not need to be a bilevel-optimal point. In fact, this point does not even need to be bilevel-feasible. See, e.g., [30], where a common heuristic for computing a big-M is shown to deliver wrong results.

The contribution of this note is twofold. First, in Section 2, we consider the hardness of verifying that a given big-M does not cut off any feasible vertex of the lower level's dual polyhedron. We show that there is no polynomial-time algorithm for this verification unless $\mathsf{P} = \mathsf{NP}$. Second, in Section 3, we show that validating that a given big-M does not cut off any optimal point of the lower level's dual problem (for any given feasible upper-level variable x) is as hard as solving the original bilevel problem. Both results together imply that there is no hope for an efficient, i.e., polynomial-time, general-purpose method for verifying or computing a correct big-M in bilevel optimization unless $\mathsf{P} = \mathsf{NP}$. Thus, our results strongly indicate that problem-specific bounds on the lower level's dual variables need to be investigated if the given bilevel problem is going to be solved using the KKT approach combined with the classical big-M linearization of KKT complementarity conditions.

2. Hardness of Bounding the Vertices of an Unbounded Polyhedron

Whenever the bilevel problem (1) is feasible, the lower-level primal and dual problem have a finite optimal solution. In particular, there is a vertex of the feasible region of the lower-level dual problem at which the optimal dual solution is attained. Thus, one way of preserving every bilevel-optimal solution in the KKT reformulation (2) is to choose a big-M such that no lower-level dual vertex is cut off. This bounding approach yields a bilevel-correct big-M. In this section, we show—even more generally—that bounding the vertices of an unbounded polyhedron is hard. This result is then applied to the lower level's dual polyhedron. Since the hardness result is mainly based on the unboundedness of this polyhedron, the question arises whether this situation frequently appears in practical LP-LP bilevel problems. It turns out that this is the case for almost all instances of bilevel test sets from the literature—which is also supported by the theoretical results in [34].

To obtain a hardness result in the Turing model of computation, we assume that all problem data are rational and thus are Turing representable. Let $P(A,b) := \{x \in \mathbb{Q}^n : Ax \le b\}$ be an unbounded polyhedron defined by $A \in \mathbb{Q}^{k\times n}$ and $b \in \mathbb{Q}^k$. For $M \in \mathbb{Q}$ and $j \in \{1,\dots,n\}$, let $Q_j(A,b,M) := \{x \in \mathbb{Q}^n : Ax \le b,\ x_j \le M\}$ be the polyhedron obtained from adding the bound $x_j \le M$ to $P(A,b)$. To validate a given big-M, we need to verify that for every $j \in \{1,\dots,n\}$ the bound $x_j \le M$ is satisfied by all vertices of $P(A,b)$. This results in the following decision problem.

Component-wise valid bound for the vertices of a polyhedron (CVBVP).
Input: $A \in \mathbb{Q}^{k\times n}$, $b \in \mathbb{Q}^k$, $j \in \{1,\dots,n\}$, $M \in \mathbb{Q}$.
Question: Does $v \in Q_j(A,b,M)$ hold for every vertex v of $P(A,b)$?

We will see in the following that validating a big-M is related to the problem of finding an optimal vertex v in an unbounded polyhedron with respect to a linear objective function $h^\top v$. If the polyhedron is bounded at least in the direction of optimization, then this problem is equivalent to linear optimization. However, in the general case of polyhedra that are unbounded in the direction of optimization, this is a difficult task. As shown in [16], the decision problem that studies the existence of a vertex of a given polyhedron such that the corresponding objective function value is larger or equal to a certain threshold K is strongly NP-complete. The proof is based on a reduction from the Hamiltonian path problem [17, Problem GT39] and can easily be extended to the decision problem that decides whether a vertex with an objective function value strictly larger than a certain threshold exists:

Optimal vertex of a polyhedron (OVP).
Input: $A \in \mathbb{Q}^{k \times n}$, $b \in \mathbb{Q}^k$, $h \in \mathbb{Q}^n$, $K \in \mathbb{Q}$.
Question: Is there a vertex v of $P(A, b)$ with $h^\top v > K$?

As pointed out above, w.r.t. the linearization (3), we are interested in the special case $h = e_j$. The related decision problem is the following:

Component-wise optimal vertex of a polyhedron (COVP).
Input: $A \in \mathbb{Q}^{k \times n}$, $b \in \mathbb{Q}^k$, $j \in \{1, \dots, n\}$, $K \in \mathbb{Q}$.
Question: Is there a vertex v of $P(A, b)$ with $v_j > K$?

We now show that even for this subclass of instances, the decision problem is strongly NP-complete. In what follows, $\operatorname{vert}(P(A, b))$ denotes the set of vertices of the polyhedron $P(A, b)$.

Theorem 1. *COVP is strongly NP-complete.*

Proof. We prove the result for $j = 1$. For any other $j' \in \{2, \dots, n\}$, e_1 can be replaced with $e_{j'}$ in the proof.

It is clear that the problem is in NP. We prove its hardness by reduction from OVP. Let $A \in \mathbb{Q}^{k \times n}$, $b \in \mathbb{Q}^k$, $h \in \mathbb{Q}^n$, $K \in \mathbb{Q}$ be a given OVP instance and assume $h \neq 0$. Otherwise, the corresponding instance is trivial. Now take $j \in \{1, \dots, n\}$ with $h_j \neq 0$. We construct a basis of $\mathbb{Q}^n$ by replacing e_j with h. If we put h as the first basis vector, the corresponding linear transformation is given by the inverse of matrix $B = [h, e_1, \dots, e_{j-1}, e_{j+1}, \dots, e_n]$ and can be computed in polynomial time. Using this basis change, we now linearly transform the hyperplanes defining the polyhedron $P(A, b)$ and the objective function vector h of the given OVP instance.

We construct an instance of COVP by $\tilde{A} = AB^{-\top}$, $\tilde{b} = b$, $\tilde{K} = K$. Note that $B^{-1}h = e_1$ holds. It remains to show that there exists a vertex v of $P(A, b)$ with $h^\top v > K$ if and only if there exists a vertex $\tilde{v}$ of $P(\tilde{A}, \tilde{b})$ with $\tilde{v}_1 > \tilde{K}$. Let $v \in \operatorname{vert}(P(A, b))$ such that $h^\top v > K$ and define $\tilde{v} := B^\top v$. Then,

$$\tilde{A}\tilde{v} = AB^{-\top}B^\top v = Av \leq b = \tilde{b}, \quad \tilde{v}_1 = h^\top B^{-\top} B^\top v = h^\top v > K = \tilde{K}.$$

Thus, $\tilde{v} \in P(\tilde{A}, \tilde{b})$ and it is clear that $\tilde{v}$ is also a vertex of $P(A, b)$.

Conversely, let $\tilde{v} \in \operatorname{vert}(P(\tilde{A}, \tilde{b}))$ with $\tilde{v}_1 > \tilde{K}$ and define $v := B^{-\top}\tilde{v}$. Then,

$$Av = AB^{-\top}\tilde{v} = \tilde{A}\tilde{v} \leq \tilde{b} = b, \quad h^\top v = h^\top B^{-\top}\tilde{v} = \tilde{v}_1 > \tilde{K} = K.$$

Thus, v is a vertex of $P(A, b)$. □

Using problem COVP, we can deduce the complexity of CVBVP.

Theorem 2. *CVBVP is strongly coNP-complete.*

Proof. The decision problem $\overline{\text{CVBVP}}$, i.e., the complement of CVBVP, is to find a vertex $v \in \operatorname{vert}(P(A, b))$ such that $v_j > M$ holds. This is equivalent to COVP with $K = M$. □

Finally, we can state the main result of this section.

Corollary 1. *Let $A \in \mathbb{Q}^{k \times n}$, $b \in \mathbb{Q}^k$, and $M \in \mathbb{Q}$. Then, there exists no polynomial-time algorithm for checking whether*

$$\operatorname{vert}(P(A, b)) \subseteq \bigcap_{j=1}^{n} Q_j(A, b, M),$$

unless P = NP.

Proof. Assume a polynomial-time algorithm exists. Then, for every $j \in \{1, \dots, n\}$ we can efficiently decide whether $\operatorname{vert}(P(A, b)) \subseteq Q_j(A, b, M)$ holds. This implies that we can decide CVBVP in polynomial time, and thus $\mathsf{P} = \mathsf{coNP}$ must also hold. Since P is closed under taking the complement, it follows that $\mathsf{P} = \mathsf{NP}$. □

As a final remark, note that to compute the tightest possible big-M such that no vertex of $P(A, b)$ is cut off, we can set

$$M := \max_{j \in \{1,\dots,n\}} \left\{ \max_{x \in \operatorname{vert}(P(A,b))} x_j \right\}. \tag{4}$$

It is equivalent to solving COVP for $j \in \{1, \dots, n\}$ and taking the maximum value. Thus, (4) cannot be computed in polynomial time, unless $\mathsf{P} = \mathsf{NP}$.

3. Valid Bounds for Bilevel-Feasible Solutions

Recall that a big-M is bilevel-correct, if it does not cut off any bilevel-optimal solution. For this, it is sufficient to find a big-M that maintains at least one optimal lower-level dual vertex for every feasible upper-level decision. This means that, in contrast to the big-M of Section 2, we now allow to cut off lower-level dual vertices that do not correspond to an optimal solution.

Here and in what follows we denote the high-point relaxation of the bilevel problem (1) as

$$H := \{(x, y) \in \mathbb{R}^n \times \mathbb{R}^m : Ax + By \geq a,\ Cx + Dy \geq b\}$$

and the corresponding projection onto the space of x-variables is defined as

$$H_x := \{x \in \mathbb{R}^n : \exists y \text{ with } (x, y) \in H\}.$$

For the sake of simplicity, we make the following assumption.

Assumption 1. *For every upper-level decision $x \in H_x$, the lower-level problem (1c) admits a unique solution y and satisfies the linear independence constraint qualifications (LICQ) at y.*

The assumption of a unique lower-level solution is justified in this scope given that the bilevel problem becomes even more difficult to analyze otherwise; see, e.g., Chapter 7 in [12]. Moreover, the LICQ guarantees the uniqueness of the lower-level dual optimal solution for every upper-level decision $x \in H_x$; see, e.g., Chapter 12 of [28]. Let us note that the assumption that LICQ holds at the unique primal solution of the lower level can be very strong. However, we will show the hardness of choosing a big-M that does not cut off any optimal vertex of the lower level's dual polyhedron under the simplifying Assumption 1. Thus, the problem of choosing such a big-M is hard also for the situation in which Assumption 1 is dropped.

We start by introducing a validity criterion for the big-M proxy discussed in this section. To this end, define the lower-level optimal value function $\varphi(x)$ for any upper-level decision $x \in H_x$ by means of its dual as

$$\varphi(x) := \max_{\lambda} \{(b - Cx)^\top \lambda \colon D^\top \lambda = f,\ \lambda \geq 0\}. \tag{5}$$

Further, for any upper-level decision $x \in H_x$, $M \in \mathbb{R}$, and $i \in \{1, \dots, \ell\}$, let $\varphi_i(x, M)$ be the optimal value function of the lower level's dual problem with the additional bound $\lambda_i \leq M$, i.e.,

$$\varphi_i(x, M) := \max_{\lambda} \{(b - Cx)^\top \lambda \colon D^\top \lambda = f,\ \lambda \geq 0,\ \lambda_i \leq M\}, \tag{6}$$

where we formally set $\varphi_i(x, M) = -\infty$ if Problem (6) is infeasible. Under Assumption 1, all bilevel-feasible solutions remain the same after adding the big-M bounds to the lower level's dual problem if and only if for every upper-level decision $x \in H_x$

and for every $i \in \{1, \dots, \ell\}$, the lower-level optimal value stays unchanged, i.e., if $\varphi(x) = \varphi_i(x, M)$ holds.

We now collect some simple observations on these two optimal value functions that are used afterward.

Observation 1. *Given an upper-level decision $x \in H_x$ and $i \in \{1, \dots, \ell\}$, the following properties hold:*

(a) $\varphi(x) \geq \varphi_i(x, M)$ for every $M \in \mathbb{R}$.
(b) $\varphi_i(x, \cdot)$ is monotonically increasing.
(c) Suppose there exists an $M \in \mathbb{R}$ with $\varphi(x) = \varphi_i(x, M)$. Then, $\varphi(x) = \varphi_i(x, \tilde{M})$ holds for every $\tilde{M} \geq M$.

Lemma 1. *Suppose that Assumption 1 holds and let an upper-level decision $x \in H_x$ and $M = M(x) \in \mathbb{R}$ be given. Then, for every $i \in \{1, \dots, \ell\}$, $\varphi(x) = \varphi_i(x, M(x))$ holds if and only if $M(x) \geq \max\{\lambda_i^*(x) \colon i \in \{1, \dots, \ell\}\}$, where $\lambda^*(x)$ is the unique optimal solution of the lower level's dual problem (5) corresponding to x.*

Proof. If $M(x) < \max\{\lambda_i^*(x) \colon i \in \{1, \dots, \ell\}\}$, then there is an $i \in \{1, \dots, \ell\}$ such that the optimal solution of the lower level's dual problem is cut off by the bound $\lambda_i \leq M(x)$, which again is equivalent to $\varphi(x) > \varphi_i(x, M(x))$. □

In particular, this implies that for every fixed upper-level decision, we can validate a given big-M by computing the corresponding unique optimal solution of the lower level's dual problem and by verifying that it satisfies the bounds $\lambda_i \leq M$ for all $i \in \{1, \dots, \ell\}$.

For the case that all upper-level decisions are taken into account, the next result gives a necessary and sufficient condition for the property that a big-M does not cut off any bilevel-feasible point.

Theorem 3. *Let $M \in \mathbb{R}$ be given and suppose that Assumption 1 holds. Then, for every upper-level decision $x \in H_x$ and for every $i \in \{1, \dots, \ell\}$, $\varphi(x) = \varphi_i(x, M)$ holds if and only if*

$$M \geq \max_{i \in \{1, \dots, \ell\}} \left\{ \max_{x,y,\lambda} \; \{\lambda_i \colon \text{(2b)}, \text{(2c)}\} \right\}. \tag{7}$$

Proof. Observe that the first constraint of (2b) defines the domain of the upper-level decisions x, whereas the second constraint together with (2c) determine the lower-level primal-dual optimal solution (y, λ) corresponding to x. The final result then follows by Lemma 1 and Property (c) in Observation 1. □

Theorem 3 implies that validating a big-M requires optimizing different objective functions over a set of constraints that are equivalent to feasibility of the original bilevel problem. In [24], linear 0-1-feasibility has been shown to be NP-complete. It is thus possible to adapt the techniques from [2] to show the NP-completeness of LP-LP bilevel feasibility by reduction from linear 0-1-feasibility. Similarly to Corollary 1, we can thus state that there is no polynomial-time validation of a given big-M w.r.t. (7) unless P = NP. On the other hand, computing the tightest big-M w.r.t. the proxy considered in this section requires solving a maximization problem over all bilevel-feasible solutions for every $i \in \{1, \dots, \ell\}$ and taking the maximum objective value. Computing this big-M is therefore as hard as solving the initial problem and there is little hope of doing it efficiently, unless the original bilevel problem (1) can be solved in polynomial time.

4. Conclusion

Many applications of LP-LP bilevel optimization make use of the KKT reformulation of the lower-level problem together with a big-M linearization of the KKT complementarity constraints. This results in a single-level mixed-integer linear problem that can, in principle, be solved with state-of-the-art solvers. However, to guarantee bilevel feasibility of a solution obtained by this approach, one needs to validate the bilevel-correctness of the big-M that is used to bound the lower level's dual variables—a necessary task that is not always carried out in practice. In general, such a big-M is bilevel-correct if it does not cut off any bilevel-optimal point. In this note we considered two proxies for this type of correctness and proved that even validating that a given big-M does not cut off any feasible or optimal vertex of the lower level's dual polyhedron cannot be done in polynomial time unless $\mathsf{P} = \mathsf{NP}$. Both proxies abstract from upper-level optimality and, thus, are only sufficient but not necessary conditions for a big-M to be bilevel-correct. Hence, validating that a given big-M preserves all bilevel-optimal points can be expected to be at least as hard since one needs to take into account another—i.e., the upper level's—optimization problem on top of what needs to be considered for the two proxies.

Our results strongly suggest that the popular big-M approach needs to be applied very carefully. If the bilevel-correctness of the chosen big-M is not guaranteed by problem-specific insights, it cannot be formally guaranteed that the obtained "solutions" are indeed bilevel-optimal. In such cases, we suggest to better resort to exact approaches that do not rely on big-M's like, e.g., the kth best algorithm ([6] or [4, Chapter 5.3.1]) or branch-and-bound methods ([3, 22], or [4, Chapter 5.3.2]). Moreover, identifying reasonably generic sub-classes of bilevel optimization problems for which it is easy to determine a bilevel-correct big-M is subject to future research.

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Article 2

Closing the Gap in Linear Bilevel Optimization: A New Valid Primal-Dual Inequality

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SHORT COMMUNICATION

Closing the gap in linear bilevel optimization: a new valid primal-dual inequality

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Abstract

Linear bilevel optimization problems are often tackled by replacing the linear lower-level problem with its Karush–Kuhn–Tucker conditions. The resulting single-level problem can be solved in a branch-and-bound fashion by branching on the complementarity constraints of the lower-level problem's optimality conditions. While in mixed-integer single-level optimization branch-and-cut has proven to be a powerful extension of branch-and-bound, in linear bilevel optimization not too many bilevel-tailored valid inequalities exist. In this paper, we briefly review existing cuts for linear bilevel problems and introduce a new valid inequality that exploits the strong duality condition of the lower level. We further discuss strengthened variants of the inequality that can be derived from McCormick envelopes. In a computational study, we show that the new valid inequalities can help to close the optimality gap very effectively on a large test set of linear bilevel instances.

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1 The difficulty in closing the optimality gap

Roughly speaking, branch-and-bound algorithms solve mathematical optimization problems by successively finding lower and upper bounds on the optimal objective function value. This procedure progressively decreases the optimality gap, i.e., the difference of the two bounds, until it is closed and the lower and upper bound meet. For minimization problems, every primal feasible solution provides a valid upper bound on the objective function value. Lower bounds in turn are computed by solving relaxations of the original problem. While modern branch-and-bound algorithms may find good primal solutions quickly, proving optimality by closing the optimality gap might be very challenging. It is not unusual to observe solution processes similar to the dashed line in Fig. 1, which shows an exemplary evolution of the lower and upper bounds over the number of visited nodes provided by a branch-and-bound implementation. An almost optimal solution is found right at the beginning, but the lower bound improves only slowly. As a result, many branch-and-bound nodes need to be visited until the gap is closed and optimality is proved.

In mixed-integer programming, the discussed obstacle has been tackled by subsequently adding valid inequalities that cut off integer-infeasible points. In many cases, this yields tighter relaxations and ultimately delivers stronger lower bounds. Such branch-and-cut algorithms are now state-of-the-art in solving mixed-integer problems.

Linear bilevel problems, in which some variables of a linear upper-level problem need to constitute an optimal solution of a second linear optimization problem (the lower-level problem), are no exception to the behavior discussed above in general.

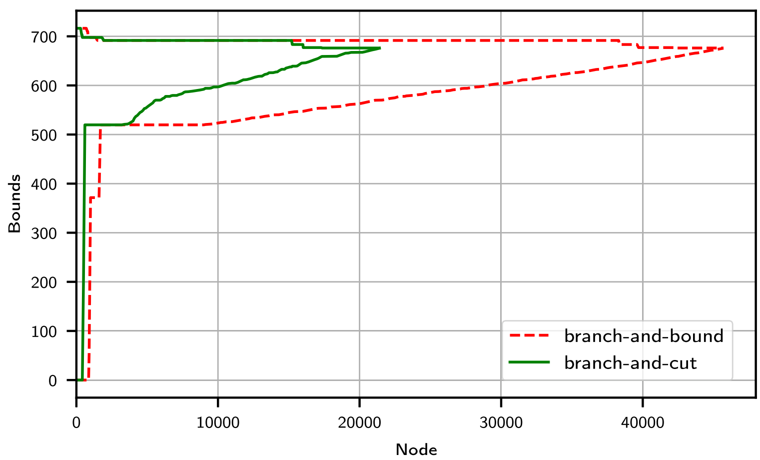

Fig. 1 Exemplary evolution of lower and upper bounds in dependence of visited nodes for a branch-and-bound (dashed) and a branch-and-cut (solid) algorithm

While bilevel-feasible points, i.e., points that satisfy all upper-level constraints and lower-level optimality, can often be found quickly [17], proving optimality is much more difficult. In fact, the dashed lines in Fig. 1 is based on a simple branch-and-bound code for linear bilevel problems applied to an exemplary instance. Similarly to mixed-integer programming, valid inequalities could be used to provide tighter relaxations of bilevel problems by cutting off bilevel-infeasible points, i.e., points that violate optimality of the lower-level problem. However, for linear bilevel problems not many tailored valid inequalities are known.

In this paper, we derive such a valid inequality for linear bilevel problems by exploiting the strong-duality condition of the lower-level problem. This primal-dual inequality turns out to be very effective for some instances. Indeed, applying it to the same instance that was used for the dashed plot in Fig. 1 yields much faster convergence; see the solid plot in Fig. 1. The lower bound increases much quicker, which results in around 20 000 visited nodes compared to roughly 45 000 nodes when the inequality is not used. We will analyze the benefit gained by the proposed valid inequality in detail in a computational study later in the paper.

The remainder of the paper is structured as follows. In Sect. 2 we formally introduce linear bilevel problems and review existing valid inequalities. Afterward, we develop a new valid inequality based on the strong-duality condition of the lower-level problem in Sect. 3 and also propose some tighter variants. In Sect. 4, we evaluate the effectiveness of the inequalities in a computational study. Finally, we conclude in Sect. 5.

2 Linear bilevel problems and valid inequalities

In this paper, we consider linear bilevel problems of the form

$$\min_{x\in\mathbb{R}^n,\, y\in\mathbb{R}^m} \quad c^\top x + d^\top y \quad \text{s.t.} \quad Ax + By \geq a, \;\; y \in \mathcal{S}(x), \tag{1}$$

where $\mathcal{S}(x)$ denotes the set of optimal solutions of the parameterized linear program

$$\max_{\bar{y}} \quad f^\top \bar{y} \quad \text{s.t.} \quad D\bar{y} \leq b - Cx, \tag{2}$$

with $c \in \mathbb{R}^n$, $d, f \in \mathbb{R}^m$, $A \in \mathbb{R}^{k\times n}$, $B \in \mathbb{R}^{k\times m}$, $a \in \mathbb{R}^k$, $C \in \mathbb{R}^{\ell\times n}$, $D \in \mathbb{R}^{\ell\times m}$, and $b \in \mathbb{R}^\ell$. The upper-level player (or leader) optimizes the upper-level problem (1) by anticipating the optimal reaction y of the lower-level player (or follower). Whenever the follower is indifferent for a given x, the set of optimal solutions $\mathcal{S}(x)$ is not a singleton. In this case, the formulation in (1) establishes the so-called optimistic solution, i.e., the leader may select any solution $y \in \mathcal{S}(x)$ that is the most favorable one for the upper-level problem; see [5]. Furthermore, throughout the paper, we make the following standard assumption (see, e.g., [1–3]) that is necessary in Sect. 3 for the derivation of a valid inequality for Problem (1).

Assumption 1 The shared constraint set

$$\Omega := \{x \in \mathbb{R}^n,\ y \in \mathbb{R}^m : Ax + By \geq a,\ Cx + Dy \leq b\}$$

is nonempty and bounded.

In general, bilevel problems are intrinsically nonconvex due to their hierarchical structure and even linear bilevel problems are known to be strongly NP-hard [14]. In addition, even checking local optimality is NP-hard; see [23]. For many real-world problems that require a bilevel or even multilevel modeling, application-specific solution techniques have been developed. This includes but is not limited to fields such as energy markets [8,13,15], pricing problems [18,19], or network interdiction problems [4,10]. In a more general setting in which no problem-specific structure can be exploited, most solution techniques resort to an equivalent single-level reformulation. For linear bilevel problems, this is typically done by replacing the lower-level problem (2) by its necessary and sufficient Karush–Kuhn–Tucker (KKT) conditions, which yields a mathematical program with complementarity constraints:

$$\min_{x,y,\lambda} \quad c^\top x + d^\top y \tag{3a}$$

$$\text{s.t.} \quad (x, y) \in \Omega, \tag{3b}$$

$$\lambda \in \Omega_D := \{\lambda \geq 0 : D^\top \lambda = f\}, \tag{3c}$$

$$\lambda^\top (b - Cx - Dy) \leq 0. \tag{3d}$$

This reformulation was first mentioned in [12], which also contains two solution approaches exploiting the disjunctive nature of the complementarity constraints (3d). The first one is a mixed-integer linear reformulation of the KKT complementarity constraints, which requires additional binary variables and sufficiently large big-M constants. The problem can then be solved by standard mixed-integer solvers. However, big-Ms that are chosen too small can yield suboptimal or infeasible solutions [21] and verifying the correctness of a big-M constant is as hard as solving the original bilevel problem; see [16]. From today's point of view, this method should only be used if correct big-Ms can be obtained via problem-specific knowledge. The second approach mentioned in [12] overcomes this obstacle by branching directly on the complementarity constraints: for all $j = 1, \dots, \ell$, either the primal lower-level constraint is binding, i.e., $(b - Cx - Dy)_j = 0$, or $\lambda_j = 0$ holds. This approach is evaluated in more detail in [3] and improving branching rules have been proposed in [14].

One drawback of this complementarity-based branch-and-bound approach (as well as of the mixed-integer approach using big-Ms) is a weak root relaxation. The problem that is solved in the root node is Problem (3) without the complementarity constraints (3d). In this setting, dual feasibility of the lower level (3c) is completely decoupled from the primal upper- and lower-level constraints (3b). In the original problem (3), these two sets of constraints are solely coupled by the complementarity constraints (3d)—the exact same constraints are initially relaxed and branched on in a bilevel branch-and-bound algorithm. In this view, the coupling is brought back subsequently via branching. It is thus desirable to extend such bilevel branch-and-bound approaches to branch-and-cut algorithms by adding cuts that resolve the missing coupling, either already at the root node or later in the branch-and-bound tree. However, up to now, not too many bilevel-specific valid inequalities are known.

In [1], the complementarity conditions (3d) are used to derive *disjunctive cuts* that can be applied to the root node problem. For each violated complementarity constraint, solving a linear optimization problem (LP) yields such a cut. In a very small example, the usefulness of the cut is demonstrated. It is also shown that sometimes this cut couples constraints (3b) and (3c) and sometimes it does not.

In [2], three root node cuts are presented that can be derived from the solution of the root node problem. The first one is a *Gomory-like cut*. For each violated complementarity constraint of the lower level, two inequalities can be derived. One of them is acting on the primal upper- and lower-level variables and the other one on the dual lower-level variables. At least one of the two inequalities must be valid and is actually a cut. Since the valid one is not known, both inequalities are added to the problem and a binary switching variable is used to select the valid inequality. In this light, the two inequalities add a rather implicit coupling of the constraints (3b) and (3c). Another variant are so-called *extended cuts* that, similar to the Gomory-like cuts, also involve binary switching variables. However, it is noted that these cuts are deeper than the Gomory-like cuts. One can also derive two cuts that do not involve a switching variable. These cuts are called *simple cuts* in [2]. Again, the combination of both cuts implicitly couples the primal upper as well as lower level with the dual lower level. In a small numerical study it is shown that applying a cut generation phase at the root node that adds cuts of either one of the three types outperforms pure branch-and-bound.

To the best of our knowledge no other general-purpose valid inequalities dedicated to linear bilevel problems have been published so far.

3 A new valid primal-dual inequality

All cuts reviewed in the last section have in common that they exploit the explicit disjunctive structure of the complementarity conditions. They are all derived from a single violated complementarity condition and it is not clear which violated one should be chosen to separate a cut. In this section, we derive a valid inequality for Problem (1) based on the aggregated complementarity conditions (3d). Using dual feasibility (3c), we can substitute $\lambda^\top D$ with f in (3d) to obtain

$$\lambda^\top b - \lambda^\top C x - f^\top y \leq 0. \tag{4}$$

This is exactly the strong-duality condition of the lower-level problem (2), as shown in the following. For a fixed upper-level decision x, the dual to the lower-level problem (2) is given by

$$\min_{\lambda \in \Omega_D} \quad \lambda^\top (b - Cx). \tag{5}$$

For every primal-dual feasible point (y, λ), weak duality

$$\lambda^\top b - \lambda^\top Cx - f^\top y \geq 0$$

holds. Thus, every primal-dual feasible point satisfying Inequality (4) fulfills the strong-duality equation and is primal-dual optimal for the lower level. An alternative formulation of the single-level reformulation (3) can hence be obtained by replacing the KKT complementarity condition (3d) with the strong duality condition (4). The main drawback of this approach is the bilinear term $\lambda^\top Cx$ of primal upper-level and dual lower-level variables. When considering only integer linking variables, as, e.g., in [25], linearizations can be applied yielding mixed-integer linear reformulations. Here, however, we study purely continuous bilevel problems. Thus, this bilinear term cannot be reformulated in a mixed-integer linear way as opposed to the KKT complementarity condition (3d).

Still, the strong duality inequality can be used to derive a valid inequality for Problem (3). A straightforward idea is to relax the nonconvex term $\lambda^\top Cx$ by replacing each term $C_{i\cdot}x$ in (4) with an upper bound $C_i^+ \geq C_{i\cdot}x$, where $C_{i\cdot}$ denotes the ith row of C. This yields the inequality

$$\lambda^\top b - \lambda^\top C^+ - f^\top y \leq 0, \tag{6}$$

where C^+ denotes the vector of upper bounds C_i^+. The rationale behind this inequality is very simple and the inequality is obviously valid. Despite, or even because of its simplicity, this inequality can be very useful. It explicitly couples the primal lower-level variable y to the dual lower-level variable λ—a coupling that is missing in the root node problem of branch-and-bound approaches. The bounds C_i^+ can be obtained, e.g., from variable bounds on x. While this approach is cheap from a computational point of view, it may result in weak inequalities depending on the tightness of the bounds on x. Stronger bounds C_i^+ can be computed with the auxiliary LPs

$$C_i^+ := \max_{x,y,\lambda} \quad C_{i\cdot}x \quad \text{s.t.} \quad (x, y, \lambda) \in \Omega \times \Omega_D, \; (x, y, \lambda) \in \mathcal{C}, \tag{7}$$

where $\mathcal{C}$ is a constraint set containing already added valid inequalities of type (6) and might be empty. This problem is bounded due to Assumption 1, such that finite bounds C_i^+ exist. In addition to the root node, Inequality (6) can also be added at any node u deeper in the branch-and-bound tree, where the bound C_i^+ is potentially tighter due to branching or previously added inequalities of type (6). This yields tighter inequalities that are locally valid for the subtree rooted at node u. Besides already added (locally) valid inequalities, the set $\mathcal{C}$ then also contains branching decisions, and $\mathcal{C}$ and C_i^+ in (7) both depend on the current branch-and-bound node u. For the ease of presentation, we omit an index u for $\mathcal{C}$ and C_i^+, because this dependence will always be clear from the context. We discuss implementation details such as the timing of the generation of valid inequalities (6) or the derivation of the bounds C_i^+ in Sect. 4, where we also demonstrate the effectiveness of the inequalities in a numerical study.

Before, let us emphasize that Inequality (6) can also be derived from another perspective. Consider a general bilinear term $z = vw$ with bounds $v^- \le v \le v^+$ and $w^- \le w \le w^+$. Then, McCormick envelopes [20] provide linear under- and overestimators for $z = vw$:

$$z \ge v^+ w + v w^+ - v^+ w^+, \qquad z \ge v^- w + v w^- - v^- w^-, \tag{8a}$$
$$z \le v^- w + v w^+ - v^- w^+, \qquad z \le v^+ w + v w^- - v^+ w^-. \tag{8b}$$

This can be applied to the strong-duality condition (4). We can decompose the bilinear products $\lambda^\top C x = \sum_{i=1}^{\ell} z_i$ to obtain terms $z_i = v_i w_i$ with $v_i = \lambda_i$ and $w_i = C_{i\cdot} x$. Due to the sign in the strong-duality condition (4), only the overestimators (8b) can be used:

$$\lambda^\top b - \sum_{i=1}^{\ell} z_i - f^\top y \le 0, \tag{9a}$$
$$z_i \le \lambda_i^- C_{i\cdot} x + \lambda_i C_i^+ - \lambda_i^- C_i^+ \quad \text{for all } i = 1, \ldots, \ell, \tag{9b}$$
$$z_i \le \lambda_i^+ C_{i\cdot} x + \lambda_i C_i^- - \lambda_i^+ C_i^- \quad \text{for all } i = 1, \ldots, \ell. \tag{9c}$$

If we apply the initial bounds $\lambda_i^- = 0$ for all $i = 1, \ldots, \ell$, then (9b) simplifies to

$$z_i \le \lambda_i C_i^+. \tag{10}$$

Obviously, Inequality (6) is fulfilled if (9a) and (10) are satisfied. Contrary, when Inequality (6) is feasible, then $z_i = \lambda_i C_i^+$ is feasible for (9a) and (10) Thus, (9a) together with (10) is equivalent to Inequality (6). However, whenever tighter (local) bounds $\lambda_i^- > 0$ are available, e.g., after presolve or branching, (9a) and (9b) provide a tightening of (6). The second overestimator (9c) involves bounds $C_i^- \le C_{i\cdot} x$, which can again be obtained by variable bounds on x or by minimizing instead of maximizing in Problem (7). However, it also involves upper bounds λ_i^+ for the initially unbounded dual variables λ_i. In general, such dual upper bounds are not available so that the overestimator (9c) cannot be used. Yet, whenever a (maybe locally valid) bound for λ_i is available by chance, e.g., due to a combination of branching and node presolve, the overestimator (9c) can be used to potentially tighten the valid inequality (6). In this light, the derivation via McCormick envelopes (8) may indeed provide tighter versions of Inequality (6). While the applicability of the tighter variants of the inequality solely depends on the availability of bounds, the basic inequality (6) can always be derived. We will discuss the applicability of the tightened variants in Sect. 4.

Furthermore, one could also relax $\lambda^\top C x$ in the strong-duality inequality (4) by replacing each term $\lambda^\top C_{\cdot j}$ with an upper bound $C_j^+ \ge \lambda^\top C_{\cdot j}$, where $C_{\cdot j}$ denotes the jth column of C. We then obtain the inequality

$$\lambda^\top b - \sum_{i=j}^{n} C_j^+ x_j - f^\top y \le 0. \tag{11}$$

This inequality couples all three types of variables x, y, and λ and can also be derived from the McCormick envelopes (8) by decomposing $\lambda^\top Cx = \sum_{j=1}^n z_j$ with $z_j = v_j w_j$, $v_j = \lambda^\top C_{\cdot j}$, and $w_j = x_j$. However, Inequality (11), respectively both overestimators (8b), involve finding lower or upper bounds $C_j^\pm$ for $\lambda^\top C_{\cdot j}$. This means that every problem

$$\min_{x,y,\lambda} \quad \lambda^\top C_{\cdot j} \quad \text{s.t.} \quad (x, y, \lambda) \in \Omega \times \Omega_D, \ (x, y, \lambda) \in \mathcal{C}, \tag{12}$$

needs to be bounded to obtain finite coefficients for each x_j. The lower-level problem (2) is bounded due to Assumption 1. Thus, the feasible set Ω_D of the dual lower-level problem (5) is bounded in the direction $b - Cx$ of the dual objective function. However, this is not necessarily the case for the optimization directions $C_{\cdot j}$. In fact, preliminary computational tests revealed that no instance in our test set has the property that all problems (12) are bounded. We thus refrain from using Inequality (11) and its variants that can be derived by McCormick envelopes. Finally, note that (6) and (11) are also valid for the pessimistic version of the bilevel problem,

$$\min_{x \in \mathbb{R}^n} \max_{y \in \mathbb{R}^m} \quad c^\top x + d^\top y \quad \text{s.t.} \quad Ax + By \geq a, \ y \in \mathcal{S}(x),$$

since the lower-level problem is still given by (2). However, in order to streamline the presentation, we will stick to the discussion of the optimistic case.

4 Computational study

We now evaluate the effectiveness of the valid inequalities derived in Sect. 3 within a complementarity-based branch-and-bound framework similar to what is described in Sect. 2. All our experiments are carried out on a single thread using the C interface of CPLEX 12.10 on a compute cluster with Xeon E3-1240 v6 CPUs at 3.7 GHz and 32 GB RAM; see [22] for more details.

Our complementarity-based branch-and-bound algorithm is realized in the following way. We introduce slack variables $s_i = b_i - C_{i\cdot}x - D_{i\cdot}y \geq 0$ to the single-level reformulation (3) for every lower-level constraint. We can then rewrite the complementarity constraints (3d) using special-ordered-sets of type 1 (SOS1) for each pair (s_i, λ_i). This way, we could use the SOS1 capabilities of CPLEX to branch on the complementarity conditions. However, to have full control and information on the branching (in particular, on the set $\mathcal{C}$), we implemented our own branching and book-keeping using generic CPLEX callbacks. We branch on the most violated complementarity constraint $i \in \{1, \dots, \ell\}$ by setting either $s_i = 0$ or $\lambda_i = 0$, while leaving the node selection to CPLEX. This basic branch-and-bound procedure serves as a benchmark and is called B&B throughout this section. Interestingly, a preliminary computational study revealed that B&B already outperforms the native SOS1 branching of CPLEX.

We extend this setting to a branch-and-cut approach by subsequently adding the valid inequalities described in Sect. 3 via generic CPLEX callbacks. We therefore use the general formulation (9). This allows to add tighter inequalities whenever the

Table 1 Test set sizes

Test set	Reference	Total	Solved	Easy	Remaining
CLIQUE	[11]	60	60	0	60
IMKP	[10]	144	70	17	53
INTER-ASSIG	[6]	24	24	4	20
INTER-CLIQUE	[11]	80	80	0	80
INTER-KP	[6]	99	78	38	40
KP	[11]	450	449	358	91
XU	[9,24]	160	160	96	64

required bounds are available. In a preliminary computational study, we tested various inequalities and strategies of how and when to add the inequalities. It turned out that computing the bounds $C_i^{\pm}$ and $\lambda_i^{\pm}$ with auxiliary LPs, similar to Problem (7), provides significantly better bounds and thus tighter inequalities than using internal global and local bounds provided "for free" by CPLEX. Although time-consuming, we follow the former approach to generate the tightest inequalities possible. Our preliminary experiments also revealed that making use of the McCormick overestimators (9b) and (9c) by tightening λ_i^- and C_i^- is only beneficial for a very small fraction of tested instances and in most cases it even harms the solution process. Hence, in the remainder of this section, we only discuss results for Inequality (6), implemented as the set of inequalities (9a) and (10). In particular, we compare the following parameterizations, where $\ell \in \mathbb{N}$ denotes the number of lower-level primal constraints:

- B&B : The branch-and-bound benchmark without additional inequalities.
- C&B : The set of inequalities (9a) and (10) is added at the root node if violated.
- B&C(5) : Inequality (9a) is added at the root and the inequalities (10) are added whenever (6) is violated at a node with depth $d = p\lfloor \ell/5 \rfloor, 0 \le p \in \mathbb{N}$.
- B&C(10) : Like B&C(5) but with $d = p\lfloor \ell/10 \rfloor$.

Obviously, the separation routine is invoked twice as many times in B&C(10) compared to B&C(5).

To compare our different methods, we use linear bilevel instances described in [17]. Table 1 summarizes the sizes of different test sets. The column "reference" indicates the origin in the literature of each subset and in the column "total" we state the size of the respective test sets. Further, the column "solved" shows how many instances are solved by at least one of the above methods in a time limit of 1 h, whereas "easy" indicates how many are solved in less then 10 s by all four methods. Finally, the last column displays the remaining number instances for each test set. Note that the test set XU consists of the test sets XUWANG and XULARGE, which are constructed the same way. Furthermore, based on our preliminary computational experiments, we completely omit the test sets DENEGRE, GENERALIZED, as well as INT0SUM since they are too easy (i.e., all instances are labeled "easy") and GK, INTER-FIRE, as well as MIPLIB since they are too hard (i.e., hardly any instance is labeled "solved"). We thus obtain a total of 408 instances in Table 1. In the following, we discuss our observations w.r.t. the remaining instances in each of these different test sets. We illustrate the performance

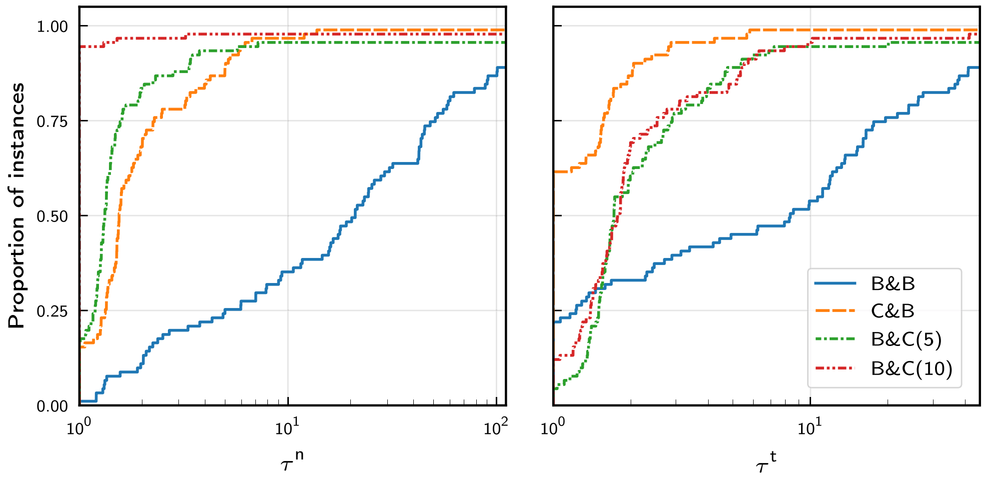

Fig. 2 Log-scaled performance profiles for branch-and-bound nodes (left) and running times (right) for all remaining KP instances; see Table 1

of the different parameterizations of our implementation using performance profiles according to [7]. For each instance i and implementation variant s, we compute the performance ratio

$$r^{\mathrm{n}}_{i,s} := \frac{n_{i,s}}{\min\{n_{i,s} : s \in S\}}$$

w.r.t. the branch-and-bound node count, where S is the set of all studied implementation variants. This means that $n_{i,s}$ is the node count of variant s on instance i. Every performance profile for node counts in this section shows the proportion of instances for which a given approach lies within a factor $\tau^{\mathrm{n}} \geq 1$ of the best approach. Similarly, we introduce τ^{t} for performance profiles w.r.t. the running times in wall-clock seconds.

It is well known that cuts often work only on a small number of instances and not throughout large and diverse test sets, in particular if they exploit a certain structure. Thus, we first discuss the impact of the valid inequalities for specific subsets of instances. It has already been shown in Fig. 1 that the application of our valid inequalities is capable of closing the optimality gap much faster compared to a pure branch-and-bound. This effect is even more pronounced for all instances of the test set CLIQUE. These instances are solved immediately once the valid inequality is added at the root node. In contrast, B&B finds the optimal solution early in the tree in most of the cases but the lower bound does not improve at all. Thus, B&B cannot solve a single instance within the time limit of 1 h. For INTER-CLIQUE, we observe a similar behavior, except that a few instances can also be solved by B&B.

On the other hand, for the test set KP, it is beneficial to also separate inequalities further down in the branch-and-bound tree. Figure 2 shows performance profiles for branch-and-bound node counts (left) and total running times (right) for these instances. We first discuss the node counts and observe that C&B yields a notable improvement over B&B. However, C&B in turn is clearly dominated by B&C(10), which needs the least branch-and-bound nodes for almost every instance. On the other hand, this comes at a

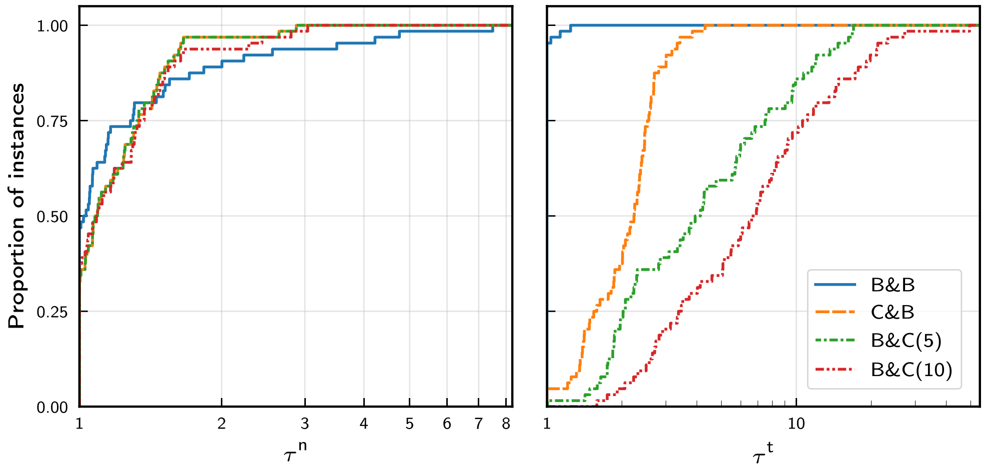

Fig. 3 Log-scaled performance profiles for branch-and-bound nodes (left) and running times (right) over remaining XU instances

certain price since the node count improvement is not significant enough to compensate the time needed to separate the additional cuts; see also the right plot in Fig. 2. Thus, C&B yields the best performance in terms of running times and dominates every other approach. The results on the test set INTER-ASSIG show similar trends w.r.t. nodes, but in contrast to KP, B&C(10) is also the best performing variant in terms of running times.

While similar trends can also be observed for the node counts for the test sets INTER-KP and IMKP, the decrease in nodes is insufficient to justify a branch-and-cut framework. In other words, B&B is dominated by every other approach in terms of node counts, but the resulting gain in running time is outweighed by cut separation, such that B&B slightly dominates the other variants in terms of running times.

Figure 3 displays performance profiles for nodes and running times restricted to the XU instances. Here, all variants perform pretty similar with respect to the node count. Since cut generation always costs computational time, it is not beneficial regarding running time to use the additional valid inequalities at all. This is especially notable for larger instances with many variables for which a large number of LPs (7) need to be solved to compute the coefficients of the cuts.

Overall, our methods are very useful on the considered instances. Figure 4 shows performance profiles for node counts and running times aggregated for all 408 instances. The branch-and-cut variants solve roughly 30 % more instances than the plain branch-and-bound procedure. All branch-and-cut variants largely outperform B&B, but there is no significant difference between the variants of the branch-and-cut method—neither in terms of node counts nor in terms of running times. To sum up, the C&B approach seems to be the best choice in general but the structure of specific instances might also lead to improved numerical results if the inequalities are added further down in the branch-and-bound tree.

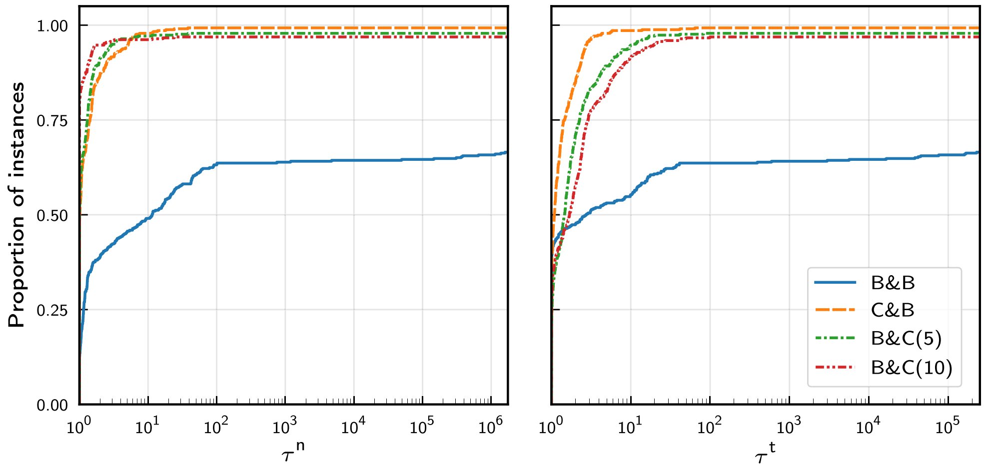

Fig. 4 Log-scaled performance profiles for branch-and-bound nodes (left) and running times (right) over all remaining instances

5 Conclusion

In this paper, we derived a new valid primal-dual inequality for linear bilevel problems based on the strong-duality condition of the linear lower-level problem. We further discussed tightened variants of the inequality resulting from McCormick envelopes and tested these inequalities in a computational study. While the latter inequalities are not beneficial in practice, the former simple variant is shown to be crucial for proving optimality for the majority of all tested instances. In fact, for many instances, adding a single inequality at the root node is sufficient to immediately close the optimality gap. For other instances, it is shown to be beneficial to add the inequality in a branch-and-cut approach further down in the branch-and-bound tree. Overall, adding the proposed valid inequalities helps to close the optimality gap much faster compared to a pure branch-and-bound algorithm and gives rise to a dedicated branch-and-cut implementation for linear bilevel problems.

While being out of scope of this short paper, we see several enhancements that could be applied within a sophisticated branch-and-cut implementation for linear bilevel problems. First, adding initial valid inequalities already before preprocessing could further improve node counts and running times. Second, in case that the inequality added in the root node does not immediately prove optimality, applying several rounds of adding valid inequalities and bound tightening could be useful. Third, whenever the separation of our inequalities yields bounds $\lambda_i^- > 0$, one could directly fix the corresponding primal lower-level constraint to be active. Finally, although our implemented branching rule already outperforms the SOS1-based branching of CPLEX, other branching and node selection rules may further improve the performance of the overall branch-and-cut implementation.

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Article 3

Bookings in the European Gas Market: Characterisation of Feasibility and Computational Complexity Results

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Bookings in the European Gas Market: Characterisation of Feasibility and Computational Complexity Results

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Abstract. As a consequence of the liberalisation of the European gas market in the last decades, gas trading and transport have been decoupled. At the core of this decoupling are so-called bookings and nominations. Bookings are special capacity right contracts that guarantee that a specified amount of gas can be supplied or withdrawn at certain entry or exit nodes of the network. These supplies and withdrawals are nominated at the day-ahead. The special property of bookings then is that they need to be feasible, i.e., every nomination that complies with the given bookings can be transported. While checking the feasibility of a nomination can typically be done by solving a mixed-integer nonlinear feasibility problem, the verification of feasibility of a set of bookings is much harder. The reason is the robust nature of feasibility of bookings – namely that for a set of bookings to be feasible, all compliant nominations, i.e., infinitely many, need to be checked for feasibility. In this paper, we consider the question of how to verify the feasibility of given bookings for a number of special cases. For our physics model we impose a steady-state potential-based flow model and disregard controllable network elements. For this case we derive a characterisation of feasible bookings, which is then used to show that the problem is in coNP for the general case but can be solved in polynomial time for linear potential-based flow models. Moreover, we present a dynamic programming approach for deciding the feasibility of a booking in tree-shaped networks even for nonlinear flow models. It turns out that the hardness of the problem mainly depends on the combination of the chosen physics model as well as the specific network structure under consideration. Thus, we give an overview over all settings for which the hardness of the problem is known and finally present a list of open problems.

1. Introduction

As a result of the liberalisation of the European gas market [22], the so-called *entry-exit* market system has been introduced [31–33]. In order to decouple trading and transport, the entry-exit market organisation specifies certain types of capacity right contracts. At the core of these contracts are the so-called *bookings* and *nominations*. In this market system, the transportation system operator (TSO) is obliged to offer the maximum amount of capacity at every node of its network, which is an upper bound on the bookable capacity. Gas traders then sign a booking contract with the TSO in which they obtain rights for maximum supplies or withdrawals at certain entry and exit nodes of the network. On a day-ahead basis, the entry and exit customers nominate the amount of gas to be supplied to or withdrawn from the network the next day. Due to the European regulation, the TSO must be able to transport every nomination that is compliant with a previously signed booking. A booking is therefore said to be feasible if and only if all booking-compliant

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nominations, i.e., infinitely many, can be transported through the network. To determine the maximum amount of capacity available at all nodes of the network, the TSO in particular needs to verify the feasibility of all possibly resulting bookings. This verification leads to very challenging mathematical problems. A mathematical model of the European entry-exit gas market system taking all these aspects into account is presented in [18]. The authors' approach has a strong economic focus, whereas we put more emphasis on physical and technical aspects of feasible bookings.

On the one hand, a lot of research has been carried out in the last decades on applying mathematical optimisation in the gas sector. Mostly, this research considered the question of verifying the feasibility of a nomination or its cost-optimal transport. In the early work [49], dynamic programming has been applied to optimise the transient and steady-state gas transport. In [7], the authors consider the cost-optimal transport problem with an application to the Belgian gas network before the European liberalisation process. As a follow-up, their techniques are updated in [2] to reflect the market situation after the liberalisation. The authors of [7] propose an extension of the simplex algorithm for the case in which gas physics are approximated with piecewise-linear functions – an approach that has been also used in, e.g., [8, 29]. As an extension, piecewise-linear relaxations have been applied in many other articles like [12–16]. A collection of solution techniques for checking the feasibility of a nomination has been discussed in the recent book [26]. Besides piecewise linearisation techniques, there (and in related work) the authors also consider NLP [44–46] and MPEC approaches [3, 38, 41–43]. In [4], simulation and optimisation techniques are combined to determine the configuration of steady-state gas flow networks. For further details on gas transport literature, we refer the reader to the recent survey [34] and the references therein.

On the other hand, there is much less mathematical literature on bookings. The problem of verifying the feasibility of a set of bookings is harder, because by definition the verification of feasible nominations has to be solved as a sub-problem. An additional difficulty is the robust nature of bookings: To certify the feasibility of a set of bookings, we need to verify that infinitely many nominations can be transported through the network. First attempts to study feasible bookings are proposed in [9, 26, 28, 48]. Given a single entry node and several exit nodes, in [17] the authors quantify the probability of booking-compliant nominations under the assumption that the exit loads follow a joint Gaussian distribution. They propose methods to validate bookings with respect to the most likely nominations. The complexity of verifying the feasibility of bookings has also been studied in the PhD thesis [21]. It is shown that the problem is coNP-complete on general networks if flows are modelled using the classical linear flow model. Furthermore, the author gives upper complexity bounds when the considered physical model is given by a potential-based flow. Structural properties like (non)convexity etc. of the sets of feasible nominations and bookings are established in [40]. Finally, an algorithm for solving the problem of robust discrete arc sizing is presented in [37]. Verifying the feasibility of bookings on a tree can be seen as a special case of this problem. Nonetheless, we will see that our tailored solution approach outperforms their algorithm, which applies to a more general setting. The recent work [1] studies the application of decomposable robust two-stage optimisation to gas network operation. Assuming linear models for controllable elements, the authors present solution approaches for determining a control of the network that minimises costs. They account for uncertainty of demand and supply as well as technical characteristics of networks elements in a robust framework. Finally, the problem of verifying the feasibility of a given set of bookings with a linear flow model is considered in [11], where the problem is called the reservation-allocation problem.

In this paper, we study the complexity of verifying the feasibility of given bookings. Due to the mathematical difficulty of this problem, we do not take into account any controllable elements and thus consider networks constituted of pipes only. Furthermore, we choose a rather abstract physics model by considering a steady-state *potential-based flow* model. These models have been introduced in [5] and can, besides gas flow, also be applied to model water or power transport networks [19, 39]. They are governed by Kirchhoff's first law and a special variant of the second law [24]. More precisely, mass is conserved at every node of the network and the flow on an arc is linked to potentials at the incident nodes through so-called *potential functions*. A key property of potential-based flow networks without controllable elements is the uniqueness of flows for given supplies and withdrawals. This result has been established in early works for fluid flow networks in [30] and more generally for potential-based flows in [35, 36]. It marks the key difference compared to classical linear flow models.

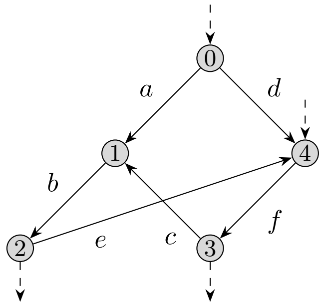
Our contribution is the following. We prove a characterisation of feasible bookings on general potential-based flow networks with arc capacities and potential bounds. This result is based on an extension of a characterisation of feasible nominations presented in [17]. As a consequence of the characterisation of feasible bookings, we are able to derive that verifying the feasibility of bookings is in coNP in general, but can be solved in polynomial time on networks with linear potential functions. Furthermore, we present a dynamic programming approach with which we can also verify in polynomial time the feasibility of bookings on tree-shaped networks with nonlinear potential functions. It turns out that the hardness of the problem thus strongly depends on the underlying flow model – i.e., the potential functions – and the network structure. We therefore conclude this paper with an overview of known complexity results for different variants of the problem and present a list of open problems.

The remainder of this paper is structured as follows. In Section 2, we introduce general notations and definitions. Section 3 establishes a characterisation of feasible bookings on general potential-based flow networks. We study the special cases of networks with linear potential functions in Section 4 and tree-shaped networks with general nonlinear potential functions in Section 5. It turns out that the hardness of verifying the feasibility of bookings strongly depends on the underlying physical flow model as well as the network structure. Thus, in the final Section 6, we give an overview of known complexity results for different combinations of these aspects. Finally, we list open problems for which the hardness is not yet known.

2. Main Definitions and Notation

The structure of a potential network is given by a directed and connected graph $G = (V, A)$. The set of nodes $V = V_+ \cup V_- \cup V_0$ is composed of the set V_+ of *entry nodes* (sources, where gas is supplied), the set V_- of *exit nodes* (sinks, where gas is withdrawn), and the set V_0 of *inner nodes*. The set of arcs A consists, in the scope of this work, only of so-called passive elements, i.e., pipes. Thus, we do not take into account any controllable elements like compressor stations or valves. For details on modelling compressor stations or other active network elements see, e.g., [38, 44] and the references therein. A network constituted of only pipes is called *passive*.

For a node $v \in V$, let $\delta^{\text{in}}(v)$ and $\delta^{\text{out}}(v)$ be the sets of arcs entering or leaving node v. Similarly, let $V^{\text{in}}(v)$ and $V^{\text{out}}(v)$ be the sets of backward and forward neighbours of v. We denote by $M \in \mathbb{R}^{V \times A}$ the *node-arc incidence matrix* of the network G. For any node $u \in V$ and arc $a \in A$, the corresponding entry is defined



$$M = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 \\ -1 & 1 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & -1 & 1 \end{bmatrix}$$

FIGURE 1. Example of a stylised gas network and its incidence matrix M. Dashed arcs indicate entry or exit nodes. The rows of M correspond to the nodes $(0, \dots, 4)$ and the columns to the arcs $(a, \dots, f)$.

by

$$m_{ua} = \begin{cases} +1, & \text{if } a = (u, v), \\ -1, & \text{if } a = (v, u), \\ 0, & \text{otherwise.} \end{cases}$$

Figure 1 shows an example of a small network, where we indicate entry and exit nodes by dashed arcs, and its corresponding incidence matrix M.

2.1. **The Physics Model.** The main motivation of this paper is to analyse structural properties of flows in gas networks. However, we will adopt a more general view of the underlying physical laws in terms of *potential-based flows*. In that way, it is possible to model flow problems with similar physical properties like electricity or water network flows. In contrast to classical flow models, potential-based flows are governed by potentials on every node of the network. Let us denote by π_v the *potential* on node $v \in V$. Due to technical limitations, the potential on every node v needs to satisfy bounds, i.e.,

$$0 \le \pi_v^- \le \pi_v \le \pi_v^+ \le \infty.$$

Further, let us denote the *flow* on arc $a \in A$ by q_a. For an arc $a = (u, v)$, we interpret $q_a > 0$ as flow in the direction of the arc, i.e., from u to v, and $q_a < 0$ as flow in the opposite direction. Additionally, the flow on every arc a has to satisfy given arc capacities

$$-\infty \le q_a^- \le q_a \le q_a^+ \le \infty.$$

Note that, both potential bounds and flow capacities can be infinite, such that this general setting can be easily applied to the case of unbounded potentials or uncapacitated flows.

Moreover, we are given a *potential function* for every arc $a \in A$ that is determined by technical properties of the pipe it represents. This potential function links the flow on an arc with the potentials on its endpoints. It can be defined as follows; see, e.g., [19].

Definition 1 (Potential functions)**.** The *potential function* of an arc $a \in A$ is a function

$$\Phi_a : \mathbb{R} \to \mathbb{R}$$

that satisfies the following properties:

(i) Φ_a is *continuous*,
(ii) Φ_a is *strictly increasing*, and

(iii) Φ_a is *odd*, i.e., $\Phi_a(-x) = -\Phi_a(x)$.

For the case of steady-state network flow models, flows and potentials are governed by Kirchhoff's first law and a special variant of the second law [24]. First, we have flow conservation on every node v with respect to (w.r.t.) a given supply or demand q_v^{n}:

$$\sum_{a \in \delta^{\mathrm{out}}(v)} q_a - \sum_{a \in \delta^{\mathrm{in}}(v)} q_a = q_v^{\mathrm{n}} \quad \text{for all } v \in V.$$

Second, the flow on arc $a = (u, v)$ is determined by the potential function of a depending on the potentials of its incident nodes u and v:

$$\pi_u - \pi_v = \Phi_a(q_a) \quad \text{for all } a = (u, v) \in A.$$

Given this link between flow and potentials, we can briefly discuss Definition 1. Whenever the flow q_a on arc $a = (u, v) \in A$ increases continuously, the difference of the potentials on both endpoints $\pi_u - \pi_v$ should also increase continuously, which is guaranteed by the first two properties of Φ_a. Furthermore, recall that the sign of q_a indicates whether there is flow in the direction of arc a or in the opposite direction. The third property of Φ_a thus ensures that the sign of the potential difference corresponds to the sign of the flow.

We can now introduce the complete model for the potential-based flow physics.

Definition 2 (Feasible potentials and flows)**.** Given supply or demand q_v^{n} for every node v, potentials π_v for every node v and flows q_a for every arc a are *feasible* if and only if they satisfy

$$\sum_{a \in \delta^{\mathrm{out}}(v)} q_a - \sum_{a \in \delta^{\mathrm{in}}(v)} q_a = q_v^{\mathrm{n}} \qquad \text{for all } v \in V, \tag{1a}$$

$$\pi_u - \pi_v = \Phi_a(q_a) \qquad \text{for all } a \in A,\ a = (u, v), \tag{1b}$$

$$\pi_v \in \left[\pi_v^-, \pi_v^+\right] \qquad \text{for all } v \in V, \tag{1c}$$

$$q_a \in \left[q_a^-, q_a^+\right] \qquad \text{for all } a \in A. \tag{1d}$$

System (1) can be rewritten in matrix notation using the node-arc incidence matrix M. We introduce the notation $q := (q_a)_{a \in A}$ to denote the vector of all arc flows. Other quantities are collected in vectors in a similar way. We then obtain

$$Mq = q^{\mathrm{n}}, \tag{2a}$$

$$M^\top \pi = \Phi(q), \tag{2b}$$

$$\pi \in \left[\pi^-, \pi^+\right], \tag{2c}$$

$$q \in \left[q^-, q^+\right]. \tag{2d}$$

Example 3. We consider three examples for which steady-state physical flows can be approximated using a potential-based flow model.

(i) *Gas transport networks*: The physical nature of gas flow is governed by partial differential equations; see e.g., [20]. If one models stationary gas flows, these relations can be approximated by an algebraic equation coupling the mass flow on the arc and the difference of squared pressures at its incident nodes; see, e.g., Chapter [10] in the book [26]. More precisely, for an arc $a = (u, v)$, it holds that

$$\exp(\delta h_u) p_u^2 - \exp(\delta h_v) p_v^2 = \Lambda_a \frac{\exp(\delta h_v) - \exp(\delta h_u)}{\delta(h_v - h_u)} |q_a| q_a,$$

where p_u is the pressure at node u, h_u is its altitude, and $\delta > 0$ is a scaling factor corresponding to the difference of the altitudes. The factor Λ_a is the so-called pressure loss factor of the pipe a, which is determined by several technical factors such as the length of the pipe, its diameter, and the roughness of the pipe's inner wall. The modelling as a potential-based flow (2) follows from identifying for any node v and any pipe $a = (u, v)$

$$\pi_v := \exp(\delta h_v) p_v^2,$$

$$\Phi_a(q_a) := \Lambda_a \frac{\exp(\delta h_v) - \exp(\delta h_u)}{\delta(h_v - h_u)} |q_a| q_a.$$

For pipes without altitude difference the above model simplifies to

$$p_u^2 - p_v^2 = \Lambda_a |q_a| q_a,$$

i.e., we have potentials $\pi_v = p_v^2$ and the potential functions are given by

$$\Phi_a(q_a) = \Lambda_a |q_a| q_a.$$

We refer to [19], where this example is discussed in depth.

(ii) *Water transport networks*: Hydraulic heads in water networks can also be interpreted as potentials. The head-loss model is then a special-case of (2) with, for any pipe a,

$$\Phi_a(q_a) := \beta_a \operatorname{sign}(q_a) |q_a|^{1.852},$$

where $\beta_a > 0$ is a pipe-specific constant. For more details on the modelling of water transport networks we refer to [27].

(iii) *Lossless DC power flow networks*: Lossless DC power flows can be modelled as a potential-based flow (2) with linear potential functions. Given a line a and its susceptance B_a, the potential function is defined as

$$\Phi_a(q_a) := \frac{1}{B_a} q_a.$$

In this case, the potentials correspond to phase angles. We refer the interested reader to [25] and the references therein for an insight to some important power flow problems. Lastly, we note that AC power flows are not captured within our framework.

2.2. **Nominations and Bookings in the European Entry-Exit Gas Market System.** In the following, we briefly sketch the notions of nominations and bookings in the European entry-exit gas market system. For more details we refer the interested reader to [18] and the references therein. In this system, the TSO signs a contract with every supply and demand customer. This contract specifies the maximum amount of flow that the customer is allowed to inject to (at entry nodes $v \in V_+$) or withdraw from (at exit nodes $v \in V_-$) the network. These capacity right contracts are called *bookings*. Furthermore, the booking at transition nodes $v \in V_0$ is always assumed to be zero. We denote by $q^{\mathrm{b}} \in \mathbb{R}^V_{\geq 0}$ the vector of all bookings in the network.

On a day-ahead basis, the customers have to commit for a *nomination* for the next day. That is, they nominate the actual amount of flow to be injected or withdrawn at the next day. We denote by $q^{\mathrm{n}} \in \mathbb{R}^V$ the vector of all nominations. We are interested in the nominations that comply with the booking q^{b}. This is formalised in the following definition.

Definition 4 (Booking-compliant nominations)**.** For a given booking $q^{\mathrm{b}} \in \mathbb{R}^V_{\geq 0}$, a nomination vector $q^{\mathrm{n}} \in \mathbb{R}^V$ is called *booking-compliant* if and only if it satisfies

$$\begin{aligned}
q^{\mathrm{n}}_v &\in \left[0, q^{\mathrm{b}}_v\right] && \text{for all } v \in V_+, && \text{(3a)}\\
q^{\mathrm{n}}_v &\in \left[-q^{\mathrm{b}}_v, 0\right] && \text{for all } v \in V_-, && \text{(3b)}\\
q^{\mathrm{n}}_v &= 0 && \text{for all } v \in V_0, && \text{(3c)}\\
\sum_{v \in V} q^{\mathrm{n}}_v &= 0. && && \text{(3d)}
\end{aligned}$$

We denote by $Q^{\mathrm{n}}(q^{\mathrm{b}})$ the polytope of booking-compliant nominations w.r.t. the booking q^{b}, as defined by System (3).

We now give the definition of a feasible nomination.

Definition 5 (Feasible nominations)**.** A given nomination $q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})$ is *feasible*, if and only if there are potentials $\pi \in \mathbb{R}^V_{\geq 0}$ and flows $q \in \mathbb{R}^A$ that satisfy System (2).

A key aspect of the European entry-exit gas market system is that the TSO has to guarantee the feasibility of every booking-compliant nomination. We thus define a feasible booking as follows.

Definition 6 (Feasible bookings)**.** A booking $q^{\mathrm{b}} \in \mathbb{R}^V_{\geq 0}$ is *feasible* if and only if every booking-compliant nomination $q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})$ is feasible.

Note that, even though we have shown several examples of potential-based flow networks in Example 3, the described notions of nominations and bookings are only used in gas transport networks. These gas networks and the underlying market system in Europe is our motivation for the analyses in this paper.

3. Characterisation of Feasible Bookings

In this section, we present a characterisation of feasible bookings, based on an extension of the characterisation of feasible nominations given in Theorem 1 of [17].

It is well-known that $\operatorname{rank}(M) = |V| - 1$ holds for connected graphs. Moreover, by choosing a reference node $0 \in V$ and a spanning tree T of G, we can decompose the incidence matrix M. Let $B := A(T)$ be the arcs of T and $N := A(G) \setminus A(T)$ the remaining arcs. By reordering the arcs of the graph, we obtain

$$M = \begin{bmatrix} m_{0B} & m_{0N} \\ M_B & M_N \end{bmatrix},$$

where

$$m_0 = \begin{pmatrix} m_{0B} & m_{0N} \end{pmatrix} \in \mathbb{R}^{\{0\} \times B}$$

is the row vector corresponding to the reference node 0. The sub-matrix $M_B \in \mathbb{R}^{(V \setminus \{0\}) \times B}$, corresponding to arcs in B after deleting the row m_0, is invertible. We call B the *basis* arcs of G and N the *non-basis* arcs. As noted above, $|V| - 1$ rows of M are linearly independent. More precisely, it holds that

$$\begin{pmatrix} m_{0B} & m_{0N} \end{pmatrix} = -e^\top \begin{bmatrix} M_B & M_N \end{bmatrix}, \tag{4}$$

where $e \in \mathbb{R}^{V \setminus \{0\}}$ is the vector of all ones.

We introduce the notation $\hat{x}_0$ to denote a vector x of node quantities without the component corresponding to the reference node 0. Using this notation, we can rewrite Constraints (2a) and (2b) as

$$M_B q_B + M_N q_N = \hat{q}_0^{\mathrm{n}},$$
$$m_{0B}^\top \pi_0 + M_B^\top \hat{\pi}_0 = \Phi_B(q_B),$$
$$m_{0N}^\top \pi_0 + M_N^\top \hat{\pi}_0 = \Phi_N(q_N).$$

Consequently, by using (4) we obtain

$$q_B = M_B^{-1}(\hat{q}_0^{\mathrm{n}} - M_N q_N), \tag{5a}$$
$$\hat{\pi}_0 = \pi_0 e + M_B^{-\top} \Phi_B \left(M_B^{-1}(\hat{q}_0^{\mathrm{n}} - M_N q_N) \right), \tag{5b}$$
$$\Phi_N(q_N) = M_N^\top M_B^{-\top} \Phi_B \left(M_B^{-1}(\hat{q}_0^{\mathrm{n}} - M_N q_N) \right). \tag{5c}$$

Constraint (5a) determines the flow on basis arcs corresponding to the spanning tree T as a function of the nomination and the flows on the non-basis arcs. Constraint (5b) yields the potential at every non-reference node as a function of the potential at the reference node 0. We introduce the function

$$g : \mathbb{R}^V \times \mathbb{R}^N \to \mathbb{R}^V$$

with

$$g(q^{\mathrm{n}}, q_N) := \begin{pmatrix} 0 \\ M_B^{-\top} \Phi_B \left(M_B^{-1}(\hat{q}_0^{\mathrm{n}} - M_N q_N) \right) \end{pmatrix}.$$

It represents the potential change caused by flow from the reference node 0 to any other node. This potential change depends both on the nomination q^{n} and the non-basis flows q_N. For the ease of presentation, we also introduce a function for the potential change between an arbitrary pair of nodes $w_1, w_2 \in V$ via

$$\Delta g_{w_1 w_2} : \mathbb{R}^V \times \mathbb{R}^N \to \mathbb{R}$$

with

$$\Delta g_{w_1 w_2}(q^{\mathrm{n}}, q_N) := g_{w_1}(q^{\mathrm{n}}, q_N) - g_{w_2}(q^{\mathrm{n}}, q_N). \tag{6}$$

Finally, Constraint (5c) ensures that the potential change between any pair of nodes is the same along all flow paths connecting the two nodes.

To verify the feasibility of the nomination q^{n}, it remains to find non-basis flows q_N satisfying Constraint (5c) as well as a reference node potential π_0 such that all additional bounds are satisfied: First, the potentials as determined by Constraint (5b) need to satisfy (2c). Second, both the basis flows q_B given by Constraint (5a) and the non-basis flows q_N need to satisfy the arc capacities (2d).

We now recap Theorem 1 in [17] in a slightly different way that will be useful for establishing the characterisation of feasible bookings later on. To do so, we also explicitly include arc capacities.

Theorem 7. Let $G = (V, A)$ be a network with given potential bounds $0 \le \pi_v^- \le \pi_v^+ \le \infty$ for every node $v \in V$ and arc capacities $-\infty \le q_a^- \le q_a^+ \le \infty$ for every arc $a \in A$. Then, a nomination $q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})$ is feasible if and only if there exist non-basis flows q_N that satisfy Constraint (5c) and

$$\Delta g_{w_1 w_2}(q^{\mathrm{n}}, q_N) \le \pi_{w_1}^+ - \pi_{w_2}^- \qquad \text{for all } w_1, w_2 \in V, \tag{7a}$$
$$q_a^- \le \left(M_B^{-1}(\hat{q}_0^{\mathrm{n}} - M_N q_N) \right)_a \le q_a^+ \qquad \text{for all } a \in B, \tag{7b}$$
$$q_a^- \le q_a \le q_a^+ \qquad \text{for all } a \in N. \tag{7c}$$

Proof. By the previous discussion, System (2) is equivalent to (5c) and

$$\begin{aligned} q_a &= \left(M_B^{-1}(\hat{q}_0^{\mathrm{n}} - M_N q_N)\right)_a && \text{for all } a \in B,\\ q_a &\in \left[q_a^-, q_a^+\right] && \text{for all } a \in A,\\ \pi_v &= \pi_0 + g_v(q^{\mathrm{n}}, q_N) && \text{for all } v \in V,\\ \pi_v &\in \left[\pi_v^-, \pi_v^+\right] && \text{for all } v \in V. \end{aligned}$$

For a fixed nomination q^{n} and non-basis flows q_N, a reference potential π_0 has to be determined such that

$$\pi_0 \in \left[\pi_v^- - g_v(q^{\mathrm{n}}, q_N), \pi_v^+ - g_v(q^{\mathrm{n}}, q_N)\right] \quad \text{for all } v \in V, \tag{8}$$

because this implies that all potentials—as given by (5b)—satisfy the bounds (2c). Using Fourier–Motzkin elimination, we eliminate the reference potential π_0 from (8). Hence, we rewrite (8) equivalently by imposing

$$\pi_{w_2}^- - g_{w_2}(q^{\mathrm{n}}, q_N) \leq \pi_{w_1}^+ - g_{w_1}(q^{\mathrm{n}}, q_N) \quad \text{for all } w_1, w_2 \in V.$$

We conclude the proof using (6). □

The latter result can be interpreted as follows. A given nomination $q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})$ is feasible if and only if we can determine non-basis flows q_N that satisfy the Constraint (5c) and Constraints (7). As soon as q_N is determined in this way, all flows and potentials are completely determined and satisfy their capacities and potential bounds, respectively. We will now see that it is always possible to determine unique non-basis flows q_N that satisfy Constraint (5c). It then needs to be checked if the other constraints are satisfied by this unique flow solution.

To prove this claim, we make use of Theorems 3 and 4 in [35]. They state that if C and D are orthogonal matrices, i.e., $CD^\top = DC^\top = 0$, and c is a given vector of supplies and demands, the system

$$\begin{aligned} Cq &= c,\\ D\Phi\left(q\right) &= 0, \end{aligned}$$

admits a unique solution $q \in \mathbb{R}^A$. As a direct corollary of this result, we obtain that flows are uniquely determined by the nomination.

Lemma 8. For every nomination $q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})$, the system formed by Constraints (5a) and (5c) admits a unique solution $q \in \mathbb{R}^A$.

Proof. Using the results of [35], it is sufficient to observe that the system can be rewritten as

$$\begin{aligned} \begin{bmatrix} M_B & M_N \end{bmatrix} q &= \hat{q}_0^{\mathrm{n}},\\ \begin{bmatrix} -M_N^\top M_B^{-\top} & \mathrm{Id} \end{bmatrix} \Phi(q) &= 0, \end{aligned}$$

where $\mathrm{Id} \in \mathbb{R}^{N \times N}$ denotes the identity matrix. Furthermore,

$$\begin{bmatrix} M_B & M_N \end{bmatrix} \begin{bmatrix} -M_B^{-1} M_N \\ \mathrm{Id} \end{bmatrix} = \begin{bmatrix} -M_N^\top M_B^{-\top} & \mathrm{Id} \end{bmatrix} \begin{bmatrix} M_B^\top \\ M_N^\top \end{bmatrix} = 0.$$ □

Note that a similar result can also be found in [47].

Example 9. The zero-nomination $q^{\mathrm{n}} = 0$ is booking-compliant for any booking q^{b} and should therefore always be feasible. The unique flows associated with q^{n} is given by Lemma 8 and we have $q = 0$. It follows that $g(0, 0) = 0$. We can rewrite Constraints (7) yielding

$$\begin{aligned} \pi^+_{w_1} &\geq \pi^-_{w_2}, && \text{for all } w_1, w_2 \in V, \\ q^-_a &\leq 0 \leq q^+_a, && \text{for all } a \in A. \end{aligned}$$

The zero-flow can then be realised by setting the potentials of all the nodes to a value $\tilde{\pi} \in \bigcap_{v \in V} [\pi^-_v, \pi^+_v]$. Hence, this is a necessary condition for a booking to be feasible. However, we will see that we do not need this additional assumption, since the infeasibility of the zero-nomination is automatically detected by the characterisation of feasible bookings that follows.

We can now give a characterisation of feasible bookings, based on Theorem 7 and Lemma 8.

Theorem 10. Let $G = (V, A)$ be a network with given potential bounds $0 \leq \pi^-_v \leq \pi^+_v \leq \infty$ for every node $v \in V$ and arc capacities $-\infty \leq q^-_a \leq q^+_a \leq \infty$ for every arc $a \in A$. Then, a booking $q^{\mathrm{b}} \in \mathbb{R}^V_{\geq 0}$ is feasible if and only if it holds that

$$\begin{aligned} \Delta g^*_{w_1 w_2} &\leq \pi^+_{w_1} - \pi^-_{w_2} && \text{for all } w_1, w_2 \in V, && \text{(9a)} \\ q^-_a \leq \underline{q}_{Ba} &\leq \overline{q}_{Ba} \leq q^+_a && \text{for all } a \in B, && \text{(9b)} \\ q^-_a \leq \underline{q}_{Na} &\leq \overline{q}_{Na} \leq q^+_a && \text{for all } a \in N, && \text{(9c)} \end{aligned}$$

with

$$\begin{aligned} \Delta g^*_{w_1 w_2} := \max_{q^{\mathrm{n}}, q_N} \quad & \Delta g_{w_1 w_2}(q^{\mathrm{n}}, q_N) && \text{(10a)} \\ \text{s.t.} \quad & \text{(5c) and } q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}}), \\ \overline{q}_{Ba} := \max_{q^{\mathrm{n}}, q_N} \quad & \left(M_B^{-1}(\hat{q}^{\mathrm{n}}_0 - M_N q_N)\right)_a && \text{(10b)} \\ \text{s.t.} \quad & \text{(5c) and } q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}}), \\ \underline{q}_{Ba} := \min_{q^{\mathrm{n}}, q_N} \quad & \left(M_B^{-1}(\hat{q}^{\mathrm{n}}_0 - M_N q_N)\right)_a && \text{(10c)} \\ \text{s.t.} \quad & \text{(5c) and } q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}}), \\ \overline{q}_{Na} := \max_{q^{\mathrm{n}}, q_N} \quad & q_a && \text{(10d)} \\ \text{s.t.} \quad & \text{(5c) and } q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}}), \\ \underline{q}_{Na} := \min_{q^{\mathrm{n}}, q_N} \quad & q_a && \text{(10e)} \\ \text{s.t.} \quad & \text{(5c) and } q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}}). \end{aligned}$$

Proof. First, assume by contradiction, that one of the constraints in (9) is violated. Without loss of generality, we consider the case in detail where there exists a pair $w_1, w_2 \in V$ such that $\Delta g^*_{w_1 w_1} > \pi^+_{w_1} - \pi^-_{w_2}$. The other cases can be handled similarly. It follows that there is a nomination $q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})$ and non-basis flows q_N satisfying Constraint (5c) with

$$\Delta g_{w_1 w_2}(q^{\mathrm{n}}, q_N) > \pi^+_{w_1} - \pi^-_{w_2}.$$

However, by Lemma 8, q_N is the unique solution of Constraint (5c). As a consequence of Theorem 7, since q_N does not satisfy Constraints (7), the booking-compliant nomination q^{n} is infeasible. It follows that the booking q^{b} is also infeasible.

Conversely, assume that $q^{\mathrm{b}} \in \mathbb{R}^V_{\geq 0}$ satisfies Constraints (9). Let $q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})$ be any booking-compliant nomination. By Lemma 8, there are unique non-basis flows q_N satisfying Constraint (5c). Furthermore, we have

$$\begin{aligned} \Delta g_{w_1 w_2}(q^{\mathrm{n}}, q_N) \leq \Delta g^*_{w_1 w_2} \leq \pi^+_{w_1} - \pi^-_{w_2} \quad & \text{for all } w_1, w_2 \in V, \\ q^-_a \leq \underline{q}_{Ba} \leq \left(M_B^{-1}(\hat{q}^{\mathrm{n}}_0 - M_N q_N)\right)_a \leq \overline{q}_{Ba} \leq q^+_a \quad & \text{for all } a \in B, \\ q^-_a \leq \underline{q}_{Na} \leq q_a \leq \overline{q}_{Na} \leq q^+_a \quad & \text{for all } a \in N. \end{aligned}$$

It follows from Theorem 7 that the nomination q^{n} is feasible. □

Note that the existence and uniqueness of non-basis flows q_N that satisfy Constraint (5c) is crucial for proving the previous theorem. In the first part of the proof, without uniqueness, we cannot be sure that there might not exist another solution q_N that could satisfy all the constraints. In particular, the only choice to be made in the problems in (10) is the nomination $q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})$ that uniquely determines the flows q_N. Therefore, optimising over the pair (q^{n}, q_N) is used to implicitly determine the non-basis flows corresponding to the nomination, since an explicit closed-form formula is not known.

The interpretation of Theorem 10 is similar to Theorem 7. For every constraint in (7), we determine a nomination that yields the largest violation, if any. We call these nominations *stressful* nominations in the following. In particular, we determine nominations that yield either large potential changes, or small and large arc flows. In order to certify the feasibility of the booking q^{b}, it remains to check whether the network state corresponding to every stressful nomination does not violate any potential bounds or flow capacities. Note, however, that in general it is non-trivial to determine stressful nominations since the optimisation problems (10) are both nonlinear and nonconvex problems.

Nonetheless, we can derive a first complexity result from Theorem 10.

Corollary 11. Verifying the feasibility of a booking $q^{\mathrm{b}} \in \mathbb{R}^V_{\geq 0}$ is in coNP.

Proof. A certificate for the infeasibility of booking q^{b} is given by a nomination $q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})$ and its corresponding non-basis flows q_N. The size of this certificate is bounded in the input size of the instance. Further, it can be verified that it is a valid certificate. We need to verify that Constraint (5c) holds. It then suffices to compute the objective values of Problems (10) corresponding to (q^{n}, q_N) and check that there is a violated constraint in (9). This verification can be achieved in polynomial time and is sufficient to show infeasibility of the booking q^{b}, since a stressful nomination yields larger (respectively smaller) objective values in Problems (10). □

As a final remark, observe that since the zero-nomination is always booking-compliant, we obtain the necessary conditions of Example 9 as a consequence of Theorem 10, because

$$\begin{aligned} 0 \leq \Delta g^*_{w_1 w_2} \quad & \text{for all } w_1, w_2 \in V, \\ \underline{q}_a \leq 0 \leq \overline{q}_a \quad & \text{for all } a \in A, \end{aligned}$$

holds.

4. General Networks with Linear Potential Functions

In this section, we study the special case of verifying the feasibility of a booking $q^{\mathrm{b}} \in \mathbb{R}^V_{\geq 0}$ on a network with linear potential functions. We thus assume potential functions of the form $\Phi_a(x) := \phi_a x$ for every arc $a \in A$. Here, ϕ_a is a given constant. The time-complexity of this problem is obtained as a direct consequence of Theorem 10.

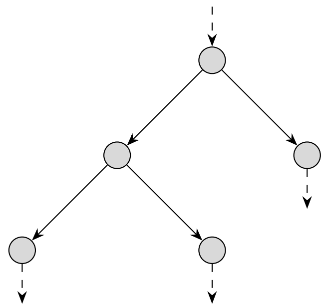


FIGURE 2. Example of a rooted out-tree.

Theorem 12. The feasibility of a booking $q^{\mathrm{b}} \in \mathbb{R}^V_{\geq 0}$ can be verified in polynomial time on general networks with linear potential functions.

Proof. Note that the set of booking-compliant nominations $Q^{\mathrm{n}}(q^{\mathrm{b}})$ is a polytope. Since all potential functions Φ are linear, the potential change function Δg and Constraint (5c) are also linear. It follows that the problems (10) are linear optimisation problems. To check whether q^{b} is feasible, we need to solve $\mathcal{O}(|V|^2)$ linear programs and check the corresponding inequalities, which yields a polynomial time algorithm. □

This result represents an interesting consequence of the characterisation of feasible bookings given by Theorem 10. It has been shown in Section 3.2.3 of [21] that verifying the feasibility of a booking on a general network is coNP-complete, if the underlying linear transport model is given by Constraints (2a) and (2d). In the more general setting that we consider here, the author also shows in Section 3.3.2 the existence of an algorithm solving the problem with a time complexity of $(4|V| + 3|A| + 2)^\kappa$ with $\kappa := (|V| + |A| + 1)(|V| + 1)$. By Theorem 12, we significantly improve this result by showing that on general networks the problem of verifying the feasibility of a booking is in P, when considering a potential-based flow with linear potential functions. The additional structure obtained by potential laws leads to existence and uniqueness of flows for every nomination, as we have shown in Lemma 8. This property is crucial for the proof of Theorem 10, which then leads to the final result in Theorem 12.

5. Tree-Shaped Networks with Nonlinear Potential Functions

In this section, we consider the special case of tree-shaped networks and nonlinear potential functions on every arc. For the remainder of this section, we therefore assume that T is a tree. In this situation, we can compute the matrix operations from Section 3 in a combinatorial way and show that the optimisation problems in (10) can be solved by dynamic programming in polynomial time. As a consequence of Theorem 10, this approach yields a closed form of the characterisation of feasible bookings on trees.

Let us first introduce some notation. The reference node 0 will be considered as the root of T. For the ease of presentation, we w.l.o.g. assume that all arcs in T are oriented away from 0, i.e., we consider rooted out-trees. Figure 2 shows an example of such a rooted out-tree. Further, we denote by L and I the set of leaves and interior nodes of T, respectively. For some $v \in V$, we denote by $T(v)$ the sub-tree of T rooted in v. Thus, we have $T = T(0)$.

Since we are considering trees, we have

$$A = B, \quad N = \emptyset, \quad M = \begin{bmatrix} m_{0B} \\ M_B \end{bmatrix}.$$

There are no non-basis arcs and all flows are basis flows, i.e., $q = q_B$. Furthermore, with $N = \emptyset$, the dependence on non-basis flows q_N in System (5) vanishes. We can thus rewrite this system as

$$q = M_B^{-1} \hat{q}_0^{\mathrm{n}}, \tag{11a}$$

$$\pi = \pi_0 e + g(q^{\mathrm{n}}), \tag{11b}$$

where we redefine the potential change function

$$g : \mathbb{R}^V \to \mathbb{R}^V$$

as

$$g(q^{\mathrm{n}}) := \begin{pmatrix} 0 \\ M_B^{-\top} \Phi_B \left(M_B^{-1} \hat{q}_0^{\mathrm{n}}\right) \end{pmatrix}.$$

As we have discussed in Section 3, $g_v(q^{\mathrm{n}})$ is the potential change caused by the flow, arising from nomination q^{n}, between the root node 0 and an arbitrary node v. Since there is a unique path between every pair of nodes in trees, Constraint (5c) does not apply. Recall that it guaranteed that the potential changes between pairs of nodes are the same for any flow path. In contrast to general networks and System (5), all flows and potentials on trees are completely determined by the nomination q^{n} and the reference potential π_0 through System (11) and does no longer depend on any non-basis flows q_N.

The flow on a given arc $a = (u, v)$ is determined by the nomination corresponding to the sub-tree of T rooted in v. It is not hard to observe that, by flow conservation (1a), any flow reaching the sub-tree has to pass through a. Therefore, the flows determined by Constraint (11a) can be obtained as given in the following lemma.

Lemma 13. Let $q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})$ be a booking-compliant nomination. For any $v \in V \setminus \{0\}$, let $\delta^{\mathrm{in}}(v) = \{a\}$, and the flow on arc a is given by

$$q_a = - \sum_{w \in V(T(v))} q_w^{\mathrm{n}}. \tag{12}$$

Proof. Take $v \in L$. Since v is a leaf, a is the only arc incident to v and $V(T(v)) = \{v\}$. Therefore, the flow conservation on v reduces to $q_a = -q_v^{\mathrm{n}}$.

Next, we consider $v \in V \setminus \{0\}$. By induction, we assume that the statement holds for every $w \in V^{\mathrm{out}}(v)$. Using flow conservation on v, we obtain

$$\sum_{w \in V^{\mathrm{out}}(v)} q_{vw} - q_a = q_v^{\mathrm{n}}.$$

By using the induction hypothesis, we then get

$$\begin{aligned} q_a &= -q_v^{\mathrm{n}} + \sum_{w \in V^{\mathrm{out}}(v)} q_{vw} \\ &= -q_v^{\mathrm{n}} + \sum_{w \in V^{\mathrm{out}}(v)} \left(- \sum_{u \in V(T(w))} q_u^{\mathrm{n}} \right) \\ &= - \sum_{u \in V(T(v))} q_u^{\mathrm{n}}. \end{aligned}$$

□

We can solve Constraint (11b) in a similar way, thus obtaining all potentials w.r.t. the reference potential. For $u, v \in V$, we define $P(u, v) \subseteq A$ to be the set of arcs corresponding to the unique undirected path between u and v in T. The potential π_w on every node w can be computed uniquely by propagation of the root node potential π_0 along the unique path $P(0, w)$.

Lemma 14. Let $q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})$ be a booking-compliant nomination. For any node $w \in V$, its potential π_w is given by

$$\pi_w = \pi_0 + \sum_{(u,v) \in P(0,w)} \Phi_{uv} \left(\sum_{l \in V(T(v))} q_l^{\mathrm{n}} \right),$$

where π_0 is the potential on the root node 0.

Proof. The statement clearly holds for $w = 0$. Thus, take $w \in V^{\mathrm{out}}(0)$. Constraint (1b) for the arc $(0, w)$ is equivalent to

$$\pi_w = \pi_0 - \Phi_{0w}(q_{0w}).$$

Recall that the potential function is odd. Using (12), we obtain the desired base case.

Next, take an arbitrary node $w \in V \setminus \{0\}$. By induction, we assume that the statement holds for $v \in V^{\mathrm{in}}(w)$. Constraint (1b) corresponding to arc (v, w) can be transformed yielding

$$\pi_w = \pi_v - \Phi_{vw}(q_{vw}) = \pi_v + \Phi_{vw} \left(\sum_{l \in V(T(w))} q_l^{\mathrm{n}} \right),$$

where the second equality again follows from (12). Applying the induction hypothesis, we get

$$\pi_w = \pi_0 + \sum_{(c,d) \in P(0,v)} \Phi_{cd} \left(\sum_{l \in V(T(d))} q_l^{\mathrm{n}} \right) + \Phi_{vw} \left(\sum_{l \in V(T(w))} q_l^{\mathrm{n}} \right),$$

which gives the desired result since $P(0, w) = P(0, v) \cup \{(v, w)\}$ holds. $\square$

As a consequence of the last lemma, the potential change from the root node 0 to any other node w is given by

$$g_w(q^{\mathrm{n}}) = \sum_{(u,v) \in P(0,w)} \Phi_{uv} \left(\sum_{l \in V(T(v))} q_l^{\mathrm{n}} \right)$$

with the usual rule that the sum over an empty set evaluates to zero, i.e., $g_0 = 0$.

For the special case of trees, we can reformulate Theorems 7 and 10. As discussed, Constraint (5c) does not apply for trees and further simplifications arise from Lemmas 13 and 14 as well as the fact that all arcs are basis arcs, i.e., $B = A$ and $N = \emptyset$.

Corollary 15. Let $T = (V, A)$ be a tree with given potential bounds $0 \le \pi_v^- \le \pi_v^+ \le \infty$ for every node $v \in V$ and arc capacities $-\infty \le q_a^- \le q_a^+ \le \infty$ for every arc $a \in A$. Then, a nomination $q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})$ is feasible if and only if

$$\Delta g_{w_1 w_2}(q^{\mathrm{n}}) \le \pi_{w_1}^+ - \pi_{w_2}^- \qquad \text{for all } w_1, w_2 \in V,$$

$$q_{uv}^- \le - \sum_{l \in V(T(v))} q_l^{\mathrm{n}} \le q_{uv}^+ \qquad \text{for all } (u, v) \in A.$$

Corollary 16. Let $T = (V, A)$ be a tree with given potential bounds $0 \leq \pi_v^- \leq \pi_v^+ \leq \infty$ for every node $v \in V$ and arc capacities $-\infty \leq q_a^- \leq q_a^+ \leq \infty$ for every arc $a \in A$. Then, a booking $q^{\mathrm{b}} \in \mathbb{R}^V_{\geq 0}$ is feasible if and only if it holds that

$$\begin{aligned} \Delta g^*_{w_1 w_2} &\leq \pi^+_{w_1} - \pi^-_{w_2} && \text{for all } w_1, w_2 \in V, \\ q^-_{uv} \leq \underline{q}_{uv} &\leq \overline{q}_{uv} \leq q^+_{uv} && \text{for all } (u, v) \in A, \end{aligned}$$

with

$$\Delta g^*_{w_1 w_2} := \max_{q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})} \Delta g_{w_1 w_2}(q^{\mathrm{n}}), \tag{13a}$$

$$\overline{q}_{uv} := \max_{q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})} - \sum_{l \in V(T(v))} q^{\mathrm{n}}_l, \tag{13b}$$

$$\underline{q}_{uv} := \min_{q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})} - \sum_{l \in V(T(v))} q^{\mathrm{n}}_l. \tag{13c}$$

Since the booking-compliant nominations $Q^{\mathrm{n}}(q^{\mathrm{b}})$ form a polytope and because the objective functions are linear, Problems (13b) and (13c) are linear optimisation problems that can be solved efficiently. However, for nonlinear potential functions Φ, Problem (13a) is a nonlinear and nonconvex optimisation problem. Fortunately, we can show that Problem (13) can be solved efficiently by dynamic programming.

Given the monotonicity of the potential functions Φ, the most stressful nomination for a given arc $(u, v) \in A$ is obtained by maximising the flow in both directions on this arc. This is formalised in the next lemma.

Lemma 17. For a given arc $(u, v) \in A$, it holds

$$\operatorname*{arg\,max}_{q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})} \Phi_{uv}\left(\sum_{l \in V(T(v))} q^{\mathrm{n}}_l\right) = \min\left\{\sum_{k \in V_- \setminus V(T(v))} q^{\mathrm{b}}_k, \sum_{k \in V_+ \cap V(T(v))} q^{\mathrm{b}}_k\right\}$$

and

$$\operatorname*{arg\,min}_{q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})} \Phi_{uv}\left(\sum_{l \in V(T(v))} q^{\mathrm{n}}_l\right) = -\min\left\{\sum_{k \in V_+ \setminus V(T(v))} q^{\mathrm{b}}_k, \sum_{k \in V_- \cap V(T(v))} q^{\mathrm{b}}_k\right\}.$$

Proof. We consider the maximisation problem in detail. The minimisation problem can then be solved similarly. Since the potential function Φ_{uv} is non-decreasing, we only need to show that

$$\operatorname*{arg\,max}_{q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})} \sum_{l \in V(T(v))} q^{\mathrm{n}}_l = \min\left\{\sum_{k \in V_- \setminus V(T(v))} q^{\mathrm{b}}_k, \sum_{k \in V_+ \cap V(T(v))} q^{\mathrm{b}}_k\right\}$$

holds. Interpreting the nomination q^{n}_l as the amount of item $l \in V(T(v))$ to be loaded, this problem can be transformed into a knapsack problem with continuous variables; see [23] for a general treatment of knapsack problems. This view has the advantage that we can solve it using a greedy algorithm as proposed in [6].

First, observe that the balance constraint $\sum_{v \in V} q^{\mathrm{n}}_v = 0$ can be written as

$$\sum_{l \in V(T(v))} q^{\mathrm{n}}_l = -\sum_{k \in V \setminus V(T(v))} q^{\mathrm{n}}_k \leq \sum_{k \in V_- \setminus V(T(v))} q^{\mathrm{b}}_k,$$

where the right-hand side of the inequality is the maximum load of the knapsack. We want to maximise the total weight of the knapsack while only considering nodes in $V(T(v))$. The variables of this problem are therefore given by q^{n}_l for $l \in V(T(v))$.

Since all the profits are positive, it is enough to only impose upper bounds derived from $Q^{\mathrm{n}}(q^{\mathrm{b}})$. Consequently, the problem we need to solve is given by

$$\begin{aligned} \max_{q^{\mathrm{n}}} \quad & \sum_{l \in V(T(v))} q^{\mathrm{n}}_l \\ \text{s.t.} \quad & \sum_{l \in V(T(v))} q^{\mathrm{n}}_l \le \sum_{k \in V_- \setminus V(T(v))} q^{\mathrm{b}}_k, \\ & q^{\mathrm{n}}_l \le q^{\mathrm{b}}_l \quad \text{for all } l \in V_+ \cap V(T(v)), \\ & q^{\mathrm{n}}_l \le 0 \quad \text{for all } l \in (V_- \cup V_0) \cap V(T(v)). \end{aligned}$$

To apply the greedy algorithm, let $V^* \subseteq V_+ \cap V\left(T(v)\right)$ be such that

$$\sum_{l \in V^*} q^{\mathrm{b}}_l \le \sum_{k \in V_- \setminus V(T(v))} q^{\mathrm{b}}_k$$

and let $w \in (V_+ \cap V\left(T(v)\right)) \setminus V^*$ such that

$$\sum_{l \in V^* \cup \{w\}} q^{\mathrm{b}}_l > \sum_{k \in V_- \setminus V(T(v))} q^{\mathrm{b}}_k$$

holds, if it exists. Otherwise, we have $V^* = V_+ \cap V\left(T(v)\right)$. The optimal solution is then given by

$$(q^{\mathrm{n}}_v)^* = \begin{cases} q^{\mathrm{b}}_v, & \text{if } v \in V^*, \\ \displaystyle\sum_{k \in V_- \setminus V(T(v))} q^{\mathrm{b}}_k - \sum_{l \in V^*} q^{\mathrm{b}}_l, & \text{if } v = w, \\ 0, & \text{if } v \in V \setminus \left(V^* \cup \{w\}\right). \end{cases}$$

This completes the proof. □

As a by-product of this result, we also obtain a closed-form expression for the maximum flow in both directions on every arc $(u, v) \in A$ by using (12). Consequently, we have

$$\bar{q}_{uv} = \min \left\{ \sum_{k \in V_+ \setminus V(T(v))} q^{\mathrm{b}}_k, \sum_{k \in V_- \cap V(T(v))} q^{\mathrm{b}}_k \right\}, \tag{14a}$$

$$\underline{q}_{uv} = -\min \left\{ \sum_{k \in V_- \setminus V(T(v))} q^{\mathrm{b}}_k, \sum_{k \in V_+ \cap V(T(v))} q^{\mathrm{b}}_k \right\}. \tag{14b}$$

In particular, the flows given in (14) can be computed in $\mathcal{O}(|V|)$ using depth-first search. With Lemma 17 at hand, we can now determine the most stressful nominations in terms of the potential change between the root node 0 and any other node $w \in V$.

Theorem 18. For all $w \in V$, we have

$$\max_{q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})} g_w(q^{\mathrm{n}}) = \sum_{(u,v) \in P(0,w)} \Phi_{uv}(-\underline{q}_{uv})$$

and

$$\min_{q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})} g_w(q^{\mathrm{n}}) = \sum_{(u,v) \in P(0,w)} \Phi_{uv}(-\bar{q}_{uv}).$$

Proof. We again consider the maximisation problem in detail. The minimisation problem can then be tackled using the same techniques. It is easy to see that

$$\max_{q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})} g_w(q^{\mathrm{n}}) \leq \sum_{(u,v) \in P(0,w)} \max_{q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})} \Phi_{uv} \left(\sum_{l \in V(T(v))} q^{\mathrm{n}}_l \right). \tag{15}$$

If we show that this inequality is satisfied with equality, the result follows from Lemma 17 and (14).

The idea to prove this is to use dynamic programming to determine a nomination $q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})$ that is optimal for all sub-problems on the right-hand side of (15). Starting with the sub-tree $T(w)$ and iterating backwards over $P(0,w)$, we fix the entries of q^{n} in such a way that the partial solution is optimal for the current sub-problem and that it is still possible to balance the nomination using nodes that have not yet been treated. Algorithm 1 presents the dynamic programming that achieves this goal.

Algorithm 1 Dynamic programming for computing $\max\{g_w(q^{\mathrm{n}}) \colon q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})\}$

Require: node $w \in V$
Ensure: $q^{\mathrm{n}} \in \arg\max\{g_w(q^{\mathrm{n}}) \colon q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})\}$
1: $v \leftarrow w$, $V^* \leftarrow \emptyset$
2: **while** $v \neq 0$ **do**
3:   **while** $l \in V_- \cap (V(T(v)) \setminus V^*)$ **and** $\sum_{k \in V_- \setminus V(T(v))} q^{\mathrm{b}}_k - \sum_{k \in V^*} q^{\mathrm{n}}_k < 0$ **do**
4:     $q^{\mathrm{n}}_l \leftarrow -\min\{q^{\mathrm{b}}_l, -(\sum_{k \in V_- \setminus V(T(v))} q^{\mathrm{b}}_k - \sum_{k \in V^*} q^{\mathrm{n}}_k)\}$
5:     $V^* \leftarrow V^* \cup \{l\}$
6:   **end while**
7:   **while** $l \in V(T(v)) \setminus V^*$ **do**
8:     **if** $l \in V_+$ **then**
9:       $q^{\mathrm{n}}_l \leftarrow \min\{q^{\mathrm{b}}_l, \sum_{k \in V_- \setminus V(T(v))} q^{\mathrm{b}}_k - \sum_{k \in V^*} q^{\mathrm{n}}_k\}$
10:     **else**
11:       $q^{\mathrm{n}}_l \leftarrow 0$
12:     **end if**
13:     $V^* \leftarrow V^* \cup \{l\}$
14:   **end while**
15:   $v \leftarrow V^{\mathrm{in}}(v)$
16: **end while**
17: **while** $l \in V_- \setminus V^*$ **do**
18:   $q^{\mathrm{n}}_l \leftarrow -\min\{q^{\mathrm{b}}_l, \sum_{k \in V^*} q^{\mathrm{n}}_k\}$
19:   $V^* \leftarrow V^* \cup \{l\}$
20: **end while**

First, consider the initial iteration where $v = w \neq 0$. The inequality in the while-condition in Line 3 does not hold since $V^* = \emptyset$. Note that the quantity

$$\rho(w) := \sum_{k \in V_- \setminus V(T(w))} q^{\mathrm{b}}_k - \sum_{k \in V^*} q^{\mathrm{n}}_k$$

is a valid upper bound for the value that the nomination q^{n}_l at a node $l \in V_+ \cap V(T(w))$ can take. It indicates the largest value that can be balanced using nodes in $V_- \setminus V(T(w))$ w.r.t. already fixed nomination values. On the other hand, the nomination q^{n}_l needs to satisfy its booking bound. We iterate over all untreated nodes in the sub-tree $T(w)$ in Line 7. We fix the nomination of nodes $l \in V_+ \cap V(T(w))$ to the largest possible value given by $\min\{q^{\mathrm{b}}_l, \rho(w)\}$.

Moreover, we fix nominations corresponding to nodes $l \in (V_- \cup V_0) \cap V(T(w))$ to 0. As a consequence,

$$\sum_{l \in V_+ \cap V(T(w))} q_l^{\mathrm{n}} = \min \left\{ \sum_{k \in V_- \setminus V(T(w))} q_k^{\mathrm{b}}, \sum_{k \in V_+ \cap V(T(w))} q_k^{\mathrm{b}} \right\}$$

holds. By Lemma 17, this construction leads to an optimal solution of the sub-problem in the right-hand side of (15) corresponding to w. We have $V^* = T(w)$ and let v be the unique predecessor of w in Line 15. This completes the while-iteration in Line 2 corresponding to node w.

If we observe that $\rho(v) \geq 0$, we proceed as in the previous case. On the other hand, if $\rho(v) < 0$ there needs to be an exit node $l \in V_- \cap (V(T(v)) \setminus V^*)$ with $q_l^{\mathrm{n}} < 0$. More precisely, while treating the nodes of $T(v)$, we need to balance the total nomination given by the values fixed over V^* that cannot be balanced in a later iteration. This is accomplished by the while-loop in Line 3. The total quantity to be withdrawn at nodes in $T(v)$ is given by $-\rho(v)$ and thus gives a lower bound for the nomination q_l^{n} for $l \in V_- \cap (V(T(v)) \setminus V^*)$. Another lower bound is again given by the booking. We thus fix the nomination q_l^{n} to $-\min\{q_l^{\mathrm{b}}, -\rho(v)\}$ while $\rho(v) < 0$. The remaining steps are identical to the initial iteration.

More generally, the following invariant holds at the end of the while-iteration in Line 2 corresponding to node v:

$$V^* = T(v) \quad \text{and} \quad \sum_{k \in V^*} q_k^{\mathrm{n}} = \min \left\{ \sum_{k \in V_+ \cap V(T(v))} q_k^{\mathrm{b}}, \sum_{k \in V_- \setminus V(T(v))} q_k^{\mathrm{b}} \right\}.$$

It thus always holds $\rho(v) \geq 0$ in Line 7.

The final while-loop in Line 17 extends the partial nomination vector to a complete balanced nomination $q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})$. By Lemma 17 and by construction, q^{n} is optimal for every sub-problem of the right-hand side of (15). Thus, equality holds, which concludes the proof. □

More generally, we can determine stressful nominations in terms of a potential change between every pair of nodes $w_1, w_2 \in V$. If we let $w \in V$ be the last common node of $P(0, w_1)$ and $P(0, w_2)$, then it is not hard to see that the potential change between w_1 and w_2 is given by

$$\Delta g_{w_1 w_2}(q^{\mathrm{n}}) = \sum_{(u,v) \in P(w,w_1)} \Phi_{uv} \left(\sum_{l \in V(T(v))} q_l^{\mathrm{n}} \right) - \sum_{(u,v) \in P(w,w_2)} \Phi_{uv} \left(\sum_{l \in V(T(v))} q_l^{\mathrm{n}} \right).$$

Since we are considering trees and by definition of w, for any pair of arcs $(u_1, v_1) \in P(w, w_1)$ and $(u_2, v_2) \in P(w, w_2)$, the sub-trees $T(v_1)$ and $T(v_2)$ do not share any nodes, i.e., $V(T(v_1)) \cap V(T(v_2)) = \emptyset$. As a consequence, both sums in the expression for $\Delta g_{w_1 w_2}(q^{\mathrm{n}})$ are separable. The idea is to maximise the first sum, similarly to Algorithm 1, and apply an adapted version of this algorithm to minimise the second sum. The resulting dynamic programming is given in Algorithm 2.

First, note that an inequality similar to (15) holds in this case as well. We show that this inequality is satisfied with equality by constructing a suitable nomination with this property. In Lines 3–17, we thus apply the maximisation techniques depicted in Algorithm 1 over sub-trees of nodes covered by the path $P(w, w_1)$. On the other hand, in Lines 19–33 we apply a "symmetric" construction for sub-trees of nodes covered by path $P(w, w_2)$. The procedure is essentially the same after exchanging entries and exits and their corresponding quantities in Algorithm 1.

Algorithm 2 Dynamic programming for computing $\Delta g^*_{w_1 w_2}$

Require: nodes $w_1, w_1 \in V$
Ensure: $q^{\mathrm{n}} \in \arg\max\{\Delta g_{w_1 w_2}(q^{\mathrm{n}})\colon q^{\mathrm{n}} \in Q^{\mathrm{n}}(q^{\mathrm{b}})\}$
$w \leftarrow$ last common node of $P(0, w_1)$ and $P(0, w_2)$
$v \leftarrow w_1, V^* \leftarrow \emptyset$
while $v \neq w$ **do**
  while $l \in V_- \cap (V(T(v)) \setminus V^*)$ **and** $\sum_{k \in V_- \setminus V(T(v))} q^{\mathrm{b}}_k - \sum_{k \in V^*} q^{\mathrm{n}}_k < 0$ **do**
    $q^{\mathrm{n}}_l \leftarrow -\min\{q^{\mathrm{b}}_l, -(\sum_{k \in V_- \setminus V(T(v))} q^{\mathrm{b}}_k - \sum_{k \in V^*} q^{\mathrm{n}}_k)\}$
    $V^* \leftarrow V^* \cup \{l\}$
  end while
  while $l \in V(T(v)) \setminus V^*$ **do**
    if $l \in V_+$ **then**
      $q^{\mathrm{n}}_l \leftarrow \min\{q^{\mathrm{b}}_l, \sum_{k \in V_- \setminus V(T(v))} q^{\mathrm{b}}_k - \sum_{k \in V^*} q^{\mathrm{n}}_k\}$
    else
      $q^{\mathrm{n}}_l \leftarrow 0$
    end if
    $V^* \leftarrow V^* \cup \{l\}$
  end while
  $v \leftarrow V^{\mathrm{in}}(v)$
end while
$v \leftarrow w_2$
while $v \neq w$ **do**
  while $l \in V_+ \cap (V(T(v)) \setminus V^*)$ **and** $\sum_{k \in V_+ \setminus V(T(v))} q^{\mathrm{b}}_k + \sum_{k \in V^*} q^{\mathrm{n}}_k < 0$ **do**
    $q^{\mathrm{n}}_l \leftarrow \min\{q^{\mathrm{b}}_l, -(\sum_{k \in V_+ \setminus V(T(v))} q^{\mathrm{b}}_k + \sum_{k \in V^*} q^{\mathrm{n}}_k)\}$
    $V^* \leftarrow V^* \cup \{l\}$
  end while
  while $l \in V(T(v)) \setminus V^*$ **do**
    if $l \in V_-$ **then**
      $q^{\mathrm{n}}_l \leftarrow -\min\{q^{\mathrm{b}}_l, \sum_{k \in V_+ \setminus V(T(v))} q^{\mathrm{b}}_k + \sum_{k \in V^*} q^{\mathrm{n}}_k\}$
    else
      $q^{\mathrm{n}}_l \leftarrow 0$
    end if
    $V^* \leftarrow V^* \cup \{l\}$
  end while
  $v \leftarrow V^{\mathrm{in}}(v)$
end while
while $l \in V_- \setminus V^*$ **do**
  $q^{\mathrm{n}}_l \leftarrow -\min\left\{q^{\mathrm{b}}_l, \sum_{k \in V^*} q^{\mathrm{n}}_k\right\}$
  $V^* \leftarrow V^* \cup \{l\}$
end while
while $l \in V_+ \setminus V^*$ **do**
  $q^{\mathrm{n}}_l \leftarrow \min\left\{q^{\mathrm{b}}_l, \sum_{k \in V^*} q^{\mathrm{n}}_k\right\}$
  $V^* \leftarrow V^* \cup \{l\}$
end while

Similarly to the proof of Theorem 18, the quantity

$$\rho(v) := \sum_{k \in V_+ \setminus V(T(v))} q^{\mathrm{b}}_k + \sum_{k \in V^*} q^{\mathrm{n}}_k$$

is a valid upper bound on the amount to be extracted at $l \in V_- \cap (V(T(v)) \setminus V^*)$, the other bound being again given by the booking. If $\rho(v) < 0$, there has to be a node $l \in V_+ \cap (V(T(v)) \setminus V^*)$ with $q_l^{\mathrm{n}} > 0$. The necessary minimal injection is then given by $-\rho(v)$. This construction leads again to an extension of partial solutions q^{n} in the sense of Lemma 17. It remains to complete the nomination q^{n} in such a way that it is balanced. This is achieved in Lines 34–41, while treating entries and exits independently. Note also that the value of the potential change between w_1 and w_2 is independent of the order in which we construct the stressful nomination. Due to the symmetry of the problem, we may obtain different stressful nominations when changing the order in which nodes are considered. However, for all these nominations, $q_a = \underline{q}_a$ for $a \in P(w, w_1)$ and $q_a = \overline{q}_a$ for $a \in P(w, w_2)$ holds. Consequently, the maximum potential change $\Delta g^*_{w_1 w_2}$ does not depend on the order. This discussion in particular also proves the following result.

Corollary 19. For given $w_1, w_2 \in V$, let $w \in V$ be the last common node of $P(0, w_1)$ and $P(0, w_2)$. Then,

$$\Delta g^*_{w_1 w_2} = - \sum_{(u,v) \in P(w,w_1)} \Phi_{uv}(\underline{q}_{uv}) + \sum_{(u,v) \in P(w,w_2)} \Phi_{uv}(\overline{q}_{uv})$$

holds.

In order to determine the most stressful nominations on a tree it is thus sufficient to generate $2\,|A|$ nominations yielding a maximum flow in both directions on every arc. As we have seen in the proof of Lemma 17, this can be done by dynamic programming for solving a continuous knapsack problem. Formally, we have the following complexity result.

Theorem 20. Verifying the feasibility of a booking $q^{\mathrm{b}} \in \mathbb{R}^V_{\geq 0}$ on trees with nonlinear potential functions is in P. More precisely, it can be done in $\mathcal{O}(|V|^2)$.

Proof. We check the feasibility of booking q^{b} using Corollary 16. To this end, we generate $\underline{q}_{uv}$ and $\overline{q}_{uv}$ for every arc $(u, v) \in A$ using (14). This is achieved in $\mathcal{O}(|V|)$. This computation thus leads to a complexity of

$$\mathcal{O}(|A| \cdot |V|) = \mathcal{O}(|V|^2).$$

To finalise the feasibility check, we need to verify $|V|^2 + 2\,|A|$ inequalities, yielding the final complexity of $\mathcal{O}(|V|^2)$. □

We finish this section with some remarks on the tree case. In [37], the authors consider the problem of robust discrete arc sizing for potential-based trees. This problem consists in determining optimal diameters for the pipes in a tree network such that a certain set of nominations is feasible. This can be used to cover the case of bookings as well. Further assuming that every pipe can take only a single diameter, namely the one in place in the existing network, we can verify the feasibility of the booking q^{b} using the approach of robust discrete arc sizing. In Lemma 4.5 of [37] it is shown that this leads to a time complexity of $\mathcal{O}(|V|^4)$. When only considering the sub-problem of verifying feasibility over trees, we have managed to improve this complexity to $\mathcal{O}(|V|^2)$. However, let us also remark that the main goal of [37] is different to ours and our setting is only contained there as a special case. Thus, it is reasonable that our tailored solution approach outperforms the one in [37].

Note also that we can restate the characterisation of feasible bookings from Corollary 16 under a closed form involving only the booking q^{b}. It is sufficient to replace the corresponding quantities by using Corollary 19 and (14). As a final remark, it is also interesting to point out that the results of this section can easily be extended to series-parallel networks, since they can be reduced to trees [19] in our potential-based setting.

6. Conclusion and Open Problems

In this paper we have studied the problem of verifying the feasibility of a set of bookings as they are used in the European entry-exit gas market system. To this end, we introduced the basic notions of feasible nominations and bookings. Then, we proved a characterisation of feasible bookings for potential-based flow models. This characterisation is based on an extension of the characterisation of feasible nominations presented in [17]. Our characterisation of feasible bookings is given in terms of inequalities on the optimal values of well-chosen optimisation problems. We applied this result to the special cases of (i) linear potential functions on general networks and (ii) nonlinear potential functions on trees. As a consequence, we showed that the feasibility of a set of bookings can be verified in polynomial time in both cases. In contrast, we have shown that the problem on general networks with nonlinear potential functions is in coNP. By these results, it has become obvious that the hardness of the problem depends both on characteristics of the physical flow model and the structure of the network.

There are still open problems since the exact border between easy and hard variants of this problem is not yet entirely known. Figure 3 summarises what is presently known regarding the problem of feasible bookings on trees and cyclic networks under different flow models.

We first discuss the upper part of the figure where a classical linear flow model is imposed for the underlying physics. It is not hard to observe that if there are no arc capacities, every balanced nomination is feasible and thus also every booking is. On the other hand, when capacities are given, it is shown in [21] that the problem is solvable in polynomial time on trees, but is coNP-complete on general, i.e., cyclic networks.

In the lower part of the figure, we illustrate cases using a potential-based flow model. Again, it is not hard to observe that every nomination and booking is feasible on an uncapacitated network without potential bounds. On the other hand, if either arc capacities or potential bounds are given the hardness depends on the nature of the potential functions and the specific structure of the network. First, we have shown in this paper that the problem can be solved in polynomial time if all potential functions are linear. This holds independently of the network structure. Second, the same polynomial time solvability applies to trees with nonlinear potential functions. On cyclic networks with nonlinear potential functions it is only known that the problem is in coNP. It remains an open question whether it is coNP-complete.

By a simple extension of the arguments given in [21] it can be shown that the problem is in P for the classical linear flow model on a single cycle. It, however, is not yet known if the problem is easy or hard for a single cycle and nonlinear potential-based flows. Finally, nothing is known – at least to the best of our knowledge – for the case of networks with controllable elements like compressors or valves.

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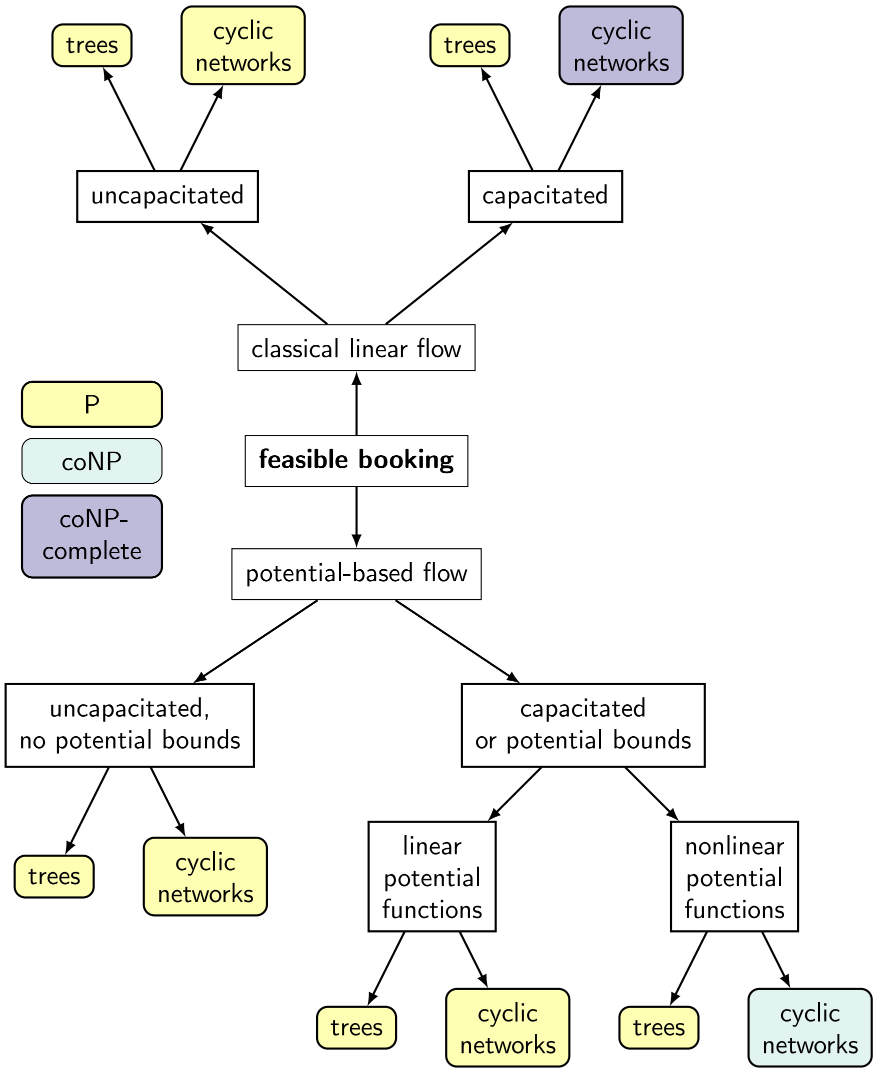

FIGURE 3. Overview of known complexity results for the problem of feasible bookings

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Article 4

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

$$\forall \ell \in N(b) : \exists y^{\psi} \in Y : \pi_u^- \le y_u^{\psi}(\ell) \le \pi_u^+, \quad u \in V. \tag{2}$$

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.,*

$$\bigcap_{u \in V} [\pi_u^-, \pi_u^+] \ne \emptyset.$$

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

$$\varphi_{w_1 w_2}(b) := \max_{\ell, q, \pi} \quad \pi_{w_1} - \pi_{w_2} \tag{3a}$$

$$\text{s.t.} \quad \text{(1a), (1b)},$$

$$0 \le \ell_u \le b_u, \quad u \in V, \tag{3b}$$

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

$$\varphi_{w_1 w_2}(b) \le \pi_{w_1}^+ - \pi_{w_2}^- \tag{4}$$

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 | NOTATIONS 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 $u' \preceq_P v'$ 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 $\ell \in N \backslash \{0\}$, 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.

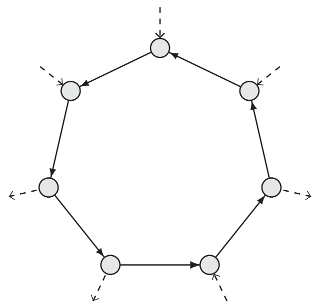

FIGURE 1 Example of a cyclic gas network. Dashed arcs to or from a node indicate entries or exits, respectively

(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 $\ell \in N \setminus \{0\}$ 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 $\ell \in N \setminus \{0\}$ 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, $w \in V \setminus \{o\}$ 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 $v' \in V^{\mathrm{r}}(v, w) \setminus \{v\}$.

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.

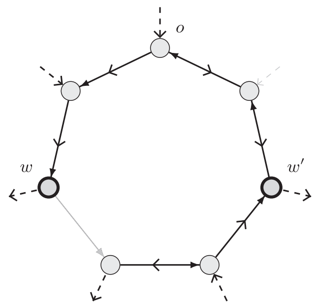

FIGURE 2 Flow directions and resulting flow-meeting points. Bold arcs indicate entry-exit activity and flow directions, whereas gray arcs indicate inactive nodes or zero arc-flow. In this example, exits w and w' are flow-meeting points

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 $u \lessdot_{\mathrm{l}} v$ instead of $u \lessdot_{P^{\mathrm{l}}(o,w)} v$. 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 $q' = q(\ell')$):*

$$\begin{aligned}
\ell' &\leq \ell, && && (9a)\\
0 &\leq q'_a && \text{for all } \ a \in A^{\mathrm{l}}(o, w), && (9b)\\
q'_a &= q_a && \text{for all } \ a \in A^{\mathrm{r}}(o, w), && (9c)\\
\Pi_{P^{\mathrm{l}}(o,x)}(q') &= \Pi_{P^{\mathrm{l}}(o,x)}(q) \geq 0, && && (9d)\\
\Pi_{P^{\mathrm{l}}(o,w)}(q') &= \Pi_{P^{\mathrm{l}}(o,w)}(q). && && (9e)
\end{aligned}$$

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

$$q'_a = \sum_{P \in \overrightarrow{\mathcal{P}}^{\mathrm{l}}_{\ell}} q(P), \quad \overrightarrow{\mathcal{P}}^{\mathrm{l}}_{\ell} := \{P \in \mathcal{P}_{\ell} : P \subseteq P^{\mathrm{l}}(u, w), \chi_a(P) = 1\}.$$

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 $(o, w) \in V_+ \times V_-$:

$$\overline{\varphi}^{ow}_{w_1 w_2}(b) := \max_{\ell, q, \pi} \quad \pi_{w_1} - \pi_{w_2} \tag{14a}$$

$$\text{s.t.} \quad \sum_{a \in \delta^{\mathrm{out}}(u)} q_a - \sum_{a \in \delta^{\mathrm{in}}(u)} q_a = \sigma_u \ell_u, \quad u \in V,$$

$$0 \leq \ell_u \leq b_u, \quad u \in V,$$

$$\pi_u - \pi_v = \Lambda_a q_a |q_a|, \quad a \in A', \tag{14b}$$

$$q_a \geq 0, \quad a \in A', \tag{14c}$$

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

$$\ell_v = 0, \quad v \in (V^{\mathrm{l}}_+(o, s^l_1) \cup V^{\mathrm{l}}_+(s^l_2, w)) \setminus \{o, s^l_1, s^l_2\},$$
$$\ell_v = b_v, \quad v \in V^{\mathrm{l}}_+(s^l_1, s^l_2) \setminus \{s^l_1, s^l_2\}.$$

(b) An exit $t^l_1 \in V^{\mathrm{l}}_-(o,w)$ exists such that

$$\ell_v = 0, \quad v \in V^{\mathrm{l}}_-(o, t^l_1) \setminus \{t^l_1\},$$
$$\ell_v = b_v, \quad v \in V^{\mathrm{l}}_-(t^l_1, w) \setminus \{t^l_1\}.$$

(c) An entry $s^r_1 \in V^{\mathrm{r}}_+(o,w)$ exists such that

$$\ell_v = b_v, \quad v \in V^{\mathrm{r}}_+(o, s^r_1) \setminus \{s^r_1\},$$
$$\ell_v = 0, \quad v \in V^{\mathrm{r}}_+(s^r_1, w) \setminus \{s^r_1\}.$$

(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

$$\ell_v = 0, \quad v \in (V^{\mathrm{r}}_-(o, t^r_1) \cup V^{\mathrm{r}}_-(t^r_2, w)) \setminus \{t^r_1, t^r_2, w\},$$
$$\ell_v = b_v, \quad v \in V^{\mathrm{r}}_-(t^r_1, t^r_2) \setminus \{t^r_1, t^r_2\}.$$

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

$$\min_{x,y} \quad f_1(\ell, x^{\preccurlyeq_\mathrm{l}}, x^{\succcurlyeq_\mathrm{l}}) + f_2(\ell, y^{\preccurlyeq_\mathrm{l}}) + f_3(\ell, x^{\succcurlyeq_\mathrm{r}}) + f_4(\ell, y^{\preccurlyeq_\mathrm{r}}, y^{\succcurlyeq_\mathrm{r}}) \tag{16a}$$

$$\text{s.t.} \quad (\ell, q, \pi) \text{ solves (14)},$$

$$Mx_v^{\preccurlyeq_\mathrm{l}} \geq \sum_{u \in V_+^\mathrm{l}(o,v)\setminus\{o\}} \ell_u, \quad v \in V_+^\mathrm{l}(o,w)\setminus\{o\}, \tag{16b}$$

$$Mx_v^{\succcurlyeq_\mathrm{l}} \geq \sum_{u \in V_+^\mathrm{l}(v,w)} \ell_u, \quad v \in V_+^\mathrm{l}(o,w)\setminus\{o\}, \tag{16c}$$

$$My_v^{\preccurlyeq_\mathrm{l}} \geq \sum_{u \in V_-^\mathrm{l}(o,v)} \ell_u, \quad v \in V_-^\mathrm{l}(o,w), \tag{16e}$$

$$Mx_v^{\succcurlyeq_\mathrm{r}} \geq \sum_{u \in V_+^\mathrm{r}(v,w)} \ell_u, \quad v \in V_+^\mathrm{r}(o,w), \tag{16e}$$

$$My_v^{\preccurlyeq_\mathrm{r}} \geq \sum_{u \in V_-^\mathrm{r}(o,v)} \ell_u, \quad v \in V_-^\mathrm{r}(o,w)\setminus\{w\}, \tag{16f}$$

$$My_v^{\succcurlyeq_\mathrm{r}} \geq \sum_{u \in V_-^\mathrm{r}(v,w)\setminus\{w\}} \ell_u, \quad v \in V_-^\mathrm{r}(o,w)\setminus\{w\}, \tag{16g}$$

$$x_v^{\preccurlyeq_\mathrm{l}}, x_v^{\succcurlyeq_\mathrm{l}}, x_v^{\succcurlyeq_\mathrm{r}}, y_v^{\preccurlyeq_\mathrm{l}}, y_v^{\preccurlyeq_\mathrm{r}}, y_v^{\succcurlyeq_\mathrm{r}} \in \{0,1\}, \quad v \in V, \tag{16h}$$

where $M = \sum_{u \in V} b_u$ and $f_1, \dots, f_4$ are continuous functions that we specify later. By Constraints (16b) and (16c), the variables $x_v^{\preccurlyeq_\mathrm{l}}$ and $x_v^{\succcurlyeq_\mathrm{l}}$ model the existence of an active entry before and after v on P^l. Similarly, Constraints (16d) ensure that $y_v^{\preccurlyeq_\mathrm{l}}$ 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 $x^{\succcurlyeq_\mathrm{r}}$, $y^{\preccurlyeq_\mathrm{r}}$, $y^{\succcurlyeq_\mathrm{r}}$. Then, the optimal value function reformulation of (16) is given by

$$\min_{\ell,q,\pi,x,y} \quad f_1(\ell, x^{\preccurlyeq_\mathrm{l}}, x^{\succcurlyeq_\mathrm{l}}) + f_2(\ell, y^{\preccurlyeq_\mathrm{l}}) + f_3(\ell, x^{\succcurlyeq_\mathrm{r}}) + f_4(\ell, y^{\preccurlyeq_\mathrm{r}}, y^{\succcurlyeq_\mathrm{r}}) \tag{17a}$$

$$\text{s.t.} \quad \text{(1a), (3b), (14b), (14c),} \tag{17b}$$

$$\text{(16b)–(16h),} \tag{17c}$$

$$\pi_{w_1} - \pi_{w_2} \geq \overline{\varphi}_{w_1 w_2}^{ow}(b). \tag{17d}$$

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

$$z := (\ell, q, \pi, x^{\preccurlyeq_\mathrm{l}}, x^{\succcurlyeq_\mathrm{l}}, x^{\succcurlyeq_\mathrm{r}}, y^{\preccurlyeq_\mathrm{l}}, y^{\preccurlyeq_\mathrm{r}}, y^{\succcurlyeq_\mathrm{r}})$$

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:

$$x_v^{\preccurlyeq_\mathrm{l}} = 1, \quad \text{if and only if an active } u \in V_+^\mathrm{l}(o,v)\setminus\{o\} \text{ exists,}$$

$$x_v^{\succcurlyeq_\mathrm{l}} = 1, \quad \text{if and only if an active } u \in V_+^\mathrm{l}(v,w)\setminus\{o\} \text{ exists,}$$

$$y_v^{\preccurlyeq_\mathrm{l}} = 1, \quad \text{if and only if an active } u \in V_-^\mathrm{l}(o,v) \text{ exists,}$$

$$x_v^{\succcurlyeq_\mathrm{r}} = 1, \quad \text{if and only if an active } u \in V_+^\mathrm{r}(v,w) \text{ exists,}$$

$$y_v^{\preccurlyeq_\mathrm{r}} = 1, \quad \text{if and only if an active } u \in V_-^\mathrm{r}(o,v)\setminus\{w\} \text{ exists,}$$

$$y_v^{\succcurlyeq_\mathrm{r}} = 1, \quad \text{if and only if an active } u \in V_-^\mathrm{r}(v,w)\setminus\{w\} \text{ exists.}$$

∎

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

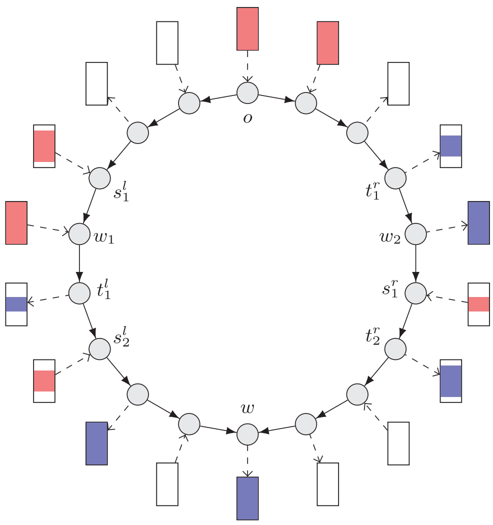

FIGURE 3 Configuration of s and t nodes if $w_1 \in P^{\mathrm{l}}(o,w)$ and $w_2 \in P^{\mathrm{r}}(o,w)$. Boxes qualitatively illustrate the amount of the booking that is nominated [Color figure can be viewed at wileyonlinelibrary.com]

- 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 $f_1, \ldots, f_4$ 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 $f_1, \ldots, f_4$, 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 $V_+^{\mathrm{l}}(i,j)\backslash\{i,j\}$, 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 $v \in V_-^{\mathrm{l}}(o,v_1)\backslash\{v_1\}$. Suppose further that z' is feasible for (17) with*

$$\ell'_{v_1} > 0, \quad \ell'_v = \ell_v, \quad u \in V_-^{\mathrm{l}}(o,w)\backslash\{v_1, w\}.$$

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 $v \in V_-^{\mathrm{l}}(o,v_1)\backslash\{v_1\}$. Hence,

$$y_i^{\preccurlyeq_{\mathrm{l}}} \sum_{v \in V_-^{\mathrm{l}}(i,w)\backslash\{i\}} (b_v - \ell_v) = 0$$

holds whenever $v_1 \in V_-^{\mathrm{l}}(i,w)\backslash\{i\}$. 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 $u \in V_+^{\mathrm{r}}(u_1,w)\backslash\{u_1\}$. Suppose further that z' is feasible for (17) with*

$$\ell'_{u_1} > 0, \quad \ell'_u = \ell_u, \quad u \in V_+^{\mathrm{r}}(o,w)\backslash\{o, u_1\}.$$

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 $u \in (V_-^{\mathrm{r}}(o,v_1) \cup V_-^{\mathrm{r}}(v_3,w))\backslash\{v_1,v_3,w\}$. Suppose further that z' is feasible for (17) with*

$$\ell'_{v_1} > 0, \quad \ell'_{v_3} > 0, \quad \ell'_u = \ell_u, \quad u \in V_-^{\mathrm{r}}(o,w)\backslash\{v_1, v_3, w\}.$$

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 $u_1, u_2, u_3 \in V_+^{\mathrm{l}}(o,w)\backslash\{o\}$ 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 $u \in V_+^{\mathrm{l}}(o,u_1)\backslash\{o,u_1\}$ and we choose u_3 such that $\ell_u = 0$ holds for all $u \in V_+^{\mathrm{l}}(u_3,w)\backslash\{u_3\}$. We now consider a flow decomposition as in Lemma 2. Due to $q \geq 0$, an exit $v_3 \in V_-^{\mathrm{l}}(u_3,w)$ 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 $v \in V_-^{\mathrm{l}}(o,v_1)\backslash\{v_1\}$ 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

$$x_{u_1}^{\preccurlyeq_{\mathrm{l}}} x_{u_3}^{\succcurlyeq_{\mathrm{l}}} \sum_{v \in V_+^{\mathrm{l}}(u_1,u_3)\backslash\{u_1,u_3\}} (b_v - \ell_v)$$

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 $\ell_{u_1} > 0, \ell_{u_2} \leq b_{u_2}, \ell_{u_3} > 0$ 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 $0 < \ell_{u_1} \leq b_{u_1}, \ell_{v_1} > 0, 0 < \ell_{v_2} \leq b_{v_2}$ 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 $q \geq 0$ in Problem (14) it follows that $\Pi_{P^r(w_1, w_2)}(q) \leq 0$ 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

$$\begin{aligned} \ell_v &= 0, \quad v \in (V_+^r(o, s_1^r) \cup V_+^r(s_2^r, w)) \setminus \{o, s_1^r, s_2^r\}, \\ \ell_v &= b_v, \quad v \in V_+^r(s_1^r, s_2^r) \setminus \{s_1^r, s_2^r\}, \end{aligned}$$

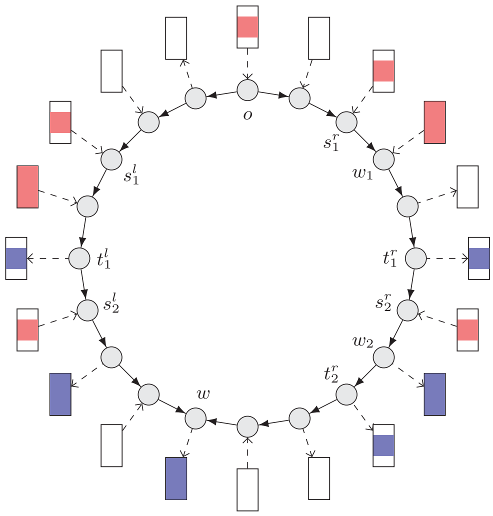

FIGURE 4 Configuration of s and t nodes with $o \preccurlyeq_r w_1 \prec_r w_2 \preccurlyeq_r w$. Boxes qualitatively illustrate the amount of the booking that is nominated [Color figure can be viewed at wileyonlinelibrary.com]

is satisfied. Figure 4 illustrates a possible node configuration. To this end, we introduce an optimization problem similar to (16), which is given by

$$\min_{\ell,q,\pi,x,y} \quad f_1(\ell, x^{\preccurlyeq_l}, x^{\succcurlyeq_l}) + f_2(\ell, y^{\preccurlyeq_l}) + f_3(\ell, x^{\preccurlyeq_r}, x^{\succcurlyeq_r}) + f_4(\ell, y^{\preccurlyeq_r}, y^{\succcurlyeq_r}) \tag{22a}$$

s.t. (1a), (3b), (14b), (14c), (16b)–(16h), (17d),

$$Mx_v^{\preccurlyeq_r} \geq \sum_{u \in V_+^r(o,v) \setminus \{o\}} \ell_u, \quad v \in V_+^r(o,v) \setminus \{o\}, \tag{22b}$$

$$x_v^{\preccurlyeq_r} \in \{0,1\}, \quad v \in V. \tag{22c}$$

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 $f_1(\ell, x^{\preccurlyeq_l}, x^{\succcurlyeq_l}) = 0$ 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 $P^l(o, w)$. Consequently, we do not change the potential difference between w_1 and w_2 due to $w_1, w_2 \in P^r(o, w)$. ∎

Lemma 31. *If z is an optimal solution of (22), then $f_2(\ell, y^{\preccurlyeq_l}) = 0$ 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 $v \in V_-^r(o, w_1)$ and $\ell_u = 0$ for all $u \in V_+^r(w_2, w)$ is satisfied.*

Proof. We choose an optimal solution z of (22) such that

$$\sum_{v \in V_-^r(o,w_1)} \ell_v + \sum_{u \in V_+^r(w_2,w)} \ell_u$$

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 $v' \in V_-^{\mathrm{r}}(o, v)\setminus\{v\}$ is satisfied. Consequently, an entry $u \in V_+^{\mathrm{r}}(o, v)$ exists such that $\ell_{u'} = 0$ holds for all $u' \in V_+^{\mathrm{r}}(o, u)\setminus\{o\}$ 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 $\epsilon > 0$ 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 $\tilde{\epsilon}$ 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 $v' \in V_-^{\mathrm{r}}(v, w)\setminus\{v, w\}$ 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 $\epsilon > 0$ and $q(P^{\mathrm{l}}(s_1^l, t_1^l))$ by $\tilde{\epsilon} > 0$. ∎

Lemma 33. *If z is an optimal solution of (22), then $f_3(\ell, x^{\preccurlyeq_{\mathrm{r}}}, x^{\succcurlyeq_{\mathrm{r}}}) = 0$ holds.*

Proof. Let z be an optimal solution of (22) that satisfies Lemma 32. By contradiction, we assume that $f_3(\ell, x^{\preccurlyeq_{\mathrm{r}}}, x^{\succcurlyeq_{\mathrm{r}}}) > 0$ holds. Lemma 17 implies that ℓ does not satisfy Property (a) w.r.t. P^{r}. Consequently, there are entries $u_1, u_2, u_3 \in V_+^{\mathrm{r}}(o, w)\setminus\{o\}$ 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 $u \in V_+^{\mathrm{r}}(o, u_1)\setminus\{o, u_1\}$ and we choose u_3 such that $\ell_u = 0$ holds for all $u \in V_+^{\mathrm{r}}(u_3, w)\setminus\{u_3\}$. We now consider a flow decomposition as in Lemma 2. Due to $q \geq 0$, an exit $v_3 \in V_-^{\mathrm{r}}(u_3, w)$ 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 $v \in V_-^{\mathrm{r}}(o, v_1)\setminus\{v_1\}$ and $q(P^{\mathrm{r}}(u_1, v_1)) > 0$. Consequently, $v_1 \preccurlyeq_{\mathrm{r}} v_3$ holds. We now distinguish two cases.

Case 1: $u_2 \preccurlyeq_{\mathrm{r}} w_1$. Due to Lemma 32, $w_1 \preccurlyeq_{\mathrm{r}} v_1$ holds. Consequently, we can decrease $q(P^{\mathrm{r}}(u_1, v_1)) > 0$ by $\epsilon > 0$ 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 $u_2 \preccurlyeq_{\mathrm{r}} w_1$. 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 $\epsilon > 0$ and increase $q(P^{\mathrm{r}}(u_2, v_3))$ by $0 < \tilde{\epsilon} \leq \epsilon$ 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 $f_4(\ell, y^{\preccurlyeq_{\mathrm{r}}}, y^{\succcurlyeq_{\mathrm{r}}}) = 0$ holds.*

Proof. Let z be an optimal solution of (22) that satisfies Lemma 32. By contradiction, we assume that $f_4(\ell, y^{\preccurlyeq_{\mathrm{r}}}, x^{\succcurlyeq_{\mathrm{r}}}) > 0$ 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 $v \in V_-^{\mathrm{l}}(v_3, w)\setminus\{v_3, w\}$. 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 $u \in V_+^{\mathrm{r}}(u_3, w)\setminus\{u_3\}$ 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 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: $v_2 \preccurlyeq_{\mathrm{r}} w_2$. Consequently, $v_1 \prec_{\mathrm{r}} v_2 \preccurlyeq_{\mathrm{r}} w_2$ holds. We can now decrease $q(P^{\mathrm{r}}(u_1, v_1))$ by $\varepsilon > 0$ and increase $q(P^{\mathrm{r}}(u_1, v_2))$ by $0 < \tilde{\varepsilon} \leq \varepsilon$ such that $\Pi_{P^{\mathrm{r}}(o,w)}$ 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 $a \in P^{\mathrm{r}}(u_1, v_1)$ and increases arc flows q_a for $a \in P^{\mathrm{r}}(v_1, v_2)$. The remaining arc flows stay the same. Hence, since $w_1 \prec_{\mathrm{r}} v_1 \prec_{\mathrm{r}} v_2 \preccurlyeq_{\mathrm{r}} w_2$ 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: $w_2 \prec_{\mathrm{r}} v_2$. Consequently, $u_3 \prec_{\mathrm{r}} w_2 \prec_{\mathrm{r}} v_2 \prec_{\mathrm{r}} v_3$ holds. We can now apply Case 2 of Lemma 28. In doing so, we keep in mind that $w_1 \prec_{\mathrm{r}} v_1$ and $w_2 \prec_{\mathrm{r}} v_2 \prec_{\mathrm{r}} v_3$ 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 $w_1, w_2 \in P^{\mathrm{r}}(o, w)$. 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 $w_2 \preccurlyeq_{\mathrm{r}} w_1$ 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 $w_1 \prec_{\mathrm{r}} w_2$ 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 $P^{\mathrm{l}}(o, w)$ and $P^{\mathrm{r}}(o, w)$. We only treat the situation corresponding to Section 5 in which $o \preccurlyeq_{\mathrm{r}} w_1 \prec_{\mathrm{r}} w_2 \preccurlyeq_{\mathrm{r}} w$ 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

$$\sum_{a \in P^{\mathrm{r}}(w_1, w_2)} \Lambda_a q_a^2 > \pi_{w_1}^+ - \pi_{w_2}^-,$$

$$\sum_{a \in P^{\mathrm{l}}(o,w)} \Lambda_a q_a^2 - \sum_{a \in P^{\mathrm{r}}(o,w)} \Lambda_a q_a^2 = 0.$$

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 $\ell_w = \ell_w^{\mathrm{l}} + \ell_w^{\mathrm{r}}$ 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

$$q_a = \begin{cases} -\displaystyle\sum_{v' \in P^{\mathrm{l}}(v,w) \setminus \{w\}} \sigma_{v'} \ell_{v'} + \ell_w^{\mathrm{l}}, & \text{if } a \in P^{\mathrm{l}}(o, w), \\ -\displaystyle\sum_{v' \in P^{\mathrm{r}}(v,w) \setminus \{w\}} \sigma_{v'} \ell_{v'} + \ell_w^{\mathrm{r}}, & \text{if } a \in P^{\mathrm{r}}(o, w). \end{cases}$$

As a consequence of the previous discussion, we need to check that the system of polynomials

$$\sum_{a=(u,v)\in P^{\mathrm{r}}(w_1,w_2)} \Lambda_a \left(- \sum_{v'\in P^{\mathrm{r}}(v,w)\setminus\{w\}} \sigma_{v'} \ell_{v'} + \ell_w^{\mathrm{r}} \right)^2 > \pi_{w_1}^{+} - \pi_{w_2}^{-}, \tag{24a}$$

$$\sum_{a=(u,v)\in P^{\mathrm{l}}(o,w)} \Lambda_a \left(- \sum_{v'\in P^{\mathrm{l}}(v,w)\setminus\{w\}} \sigma_{v'} \ell_{v'} + \ell_w^{\mathrm{l}} \right)^2$$

$$- \sum_{a=(u,v)\in P^{\mathrm{r}}(o,w)} \Lambda_a \left(- \sum_{v'\in P^{\mathrm{r}}(v,w)\setminus\{w\}} \sigma_{v'} \ell_{v'} + \ell_w^{\mathrm{r}} \right)^2 = 0, \tag{24b}$$

$$- \sum_{v'\in P^{\mathrm{l}}(v,w)\setminus\{w\}} \sigma_{v'} \ell_{v'} + \ell_w^{\mathrm{l}} \geq 0, \quad (u,v) \in P^{\mathrm{l}}, \tag{24c}$$

$$- \sum_{v'\in P^{\mathrm{r}}(v,w)\setminus\{w\}} \sigma_{v'} \ell_{v'} + \ell_w^{\mathrm{r}} \geq 0, \quad (u,v) \in P^{\mathrm{r}}, \tag{24d}$$

$$\ell_w^{\mathrm{l}} + \ell_w^{\mathrm{r}} = \ell_w, \quad \ell \in N(b), \tag{24e}$$

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 $s_1^l, s_2^l \in V_+^{\mathrm{l}}(o,w)$, $t_1^l \in V_-^{\mathrm{l}}(o,w)$, $s_1^r, s_2^r \in V_+^{\mathrm{r}}(o,w)$ as well as $t_1^r, t_2^r \in V_-^{\mathrm{r}}(o,w)$, 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

$$\ell_w = \ell_w^{\mathrm{l}} + \ell_w^{\mathrm{r}}, \quad \ell_o = -\sum_{u\in V\setminus\{o\}} \sigma_u \ell_u.$$

Fixing nomination entries either to their booking bound or to zero, as by Properties (a)–(d), it is easy to observe that $\ell_{s_1^l}, \ell_{s_2^l}, \ell_{t_1^l}, \ell_{s_1^r}, \ell_{s_2^r}, \ell_{t_1^r}, \ell_{t_2^r}, \ell_w^{\mathrm{l}}, \ell_w^{\mathrm{r}}$, 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 $u \in \{s_1^l, s_2^l, t_1^l, s_1^r, s_2^r, t_1^r, t_2^r\}$.

The number of additional constraints due to o and w depend on the configuration under consideration. If $o \notin \{s_1^l, s_1^r\}$, then the additional constraint $\ell_o = b_o$ is necessary. If $w \notin \{t_1^l, t_2^r\}$, 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 $s_1^r, s_2^r, t_1^r, t_2^r$. 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 to 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 $0 < \ell_{u_1} \leq b_{u_1}, \ell_{u_2} > 0, \ell_{v_2} > 0$ 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 $q \geq 0$, there is an entry $u_3 \in V_+^{\mathrm{r}}(o, v_3)$ with $\ell_u = 0$ for all $u \in V_+^{\mathrm{r}}(u_3, w) \setminus \{u_3\}$ 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 $\ell_{v_1} > 0, 0 < \ell_{v_2} \leq b_{v_2}, \ell_{u_3} > 0, \ell_{v_3} > 0$ 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 5

A Bilevel Optimization Approach to Decide the Feasibility of Bookings in the European Gas Market

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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 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.

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 [8] and the subsequent regulation [9] on

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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 [17, 43]. Some structural properties of bookings are analyzed in [43]. Further, the author of [17] 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 [12], 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 [24], 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 [24] or passive, single-cycle networks [25]. However, the problem is coNP-hard on passive networks in general [40]. Moreover, optimizing over the set of feasible bookings is hard even on tree-shaped networks [34]. 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 [1, 2, 33] 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 [33], 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 [3, 7] and the recent survey article [20]. In general, bilevel optimization has been successfully applied to many different problems in the context of energy networks; see [44]. 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., [18].

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 [15, 19], 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., [2], 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 [37]. 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 Section 2, we formally introduce the problem of deciding the feasibility of a booking in networks with active elements. In Section 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 Section 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 Section 5 and discuss various optimal-value-function reformulations and characterizations of feasible bookings in active networks in Section 6. We then compare our methods in a computational study in Section 7. Finally, we summarize our results and discuss possible directions for future research in Section 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 [25], 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*

$$N := \left\{ \ell \in L \colon \sum_{u \in V_+} \ell_u = \sum_{u \in V_-} \ell_u \right\}.$$

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 $N(b) := \{\ell \in N \colon \ell \leq b\}$.*

In the following, we consider stationary gas flows based on the Weymouth pressure loss equation [42]. In line with the corresponding literature [25, 34, 40], 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 [14]. For modeling active elements, a variety of different modeling approaches exist that range from simple linear to sophisticated mixed-integer nonlinear ones; see [11]. In this paper, we focus on linearly modeled active elements similar to [1]. 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 Section 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*

$$\forall \ell \in N(b) \ \exists (q, \pi, \Delta) \ \textit{satisfying} \ (1). \tag{2}$$

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 [4, 46] 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 [24]. 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 [24]. For each pair of nodes $(w_1, w_2) \in V^2$, the authors introduce the nonlinear

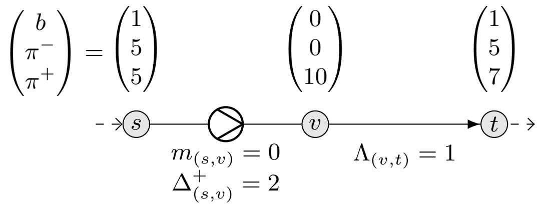

FIGURE 1. Network of the counterexample consisting of three nodes, one compressor, and one pipe, together with relevant node and arc parameters.

optimization problem

$$\varphi_{w_1 w_2}(b) := \max_{\ell,q,\pi} \quad \pi_{w_1} - \pi_{w_2} \tag{3a}$$

$$\text{s.t.} \quad \sum_{a \in \delta^{\text{out}}(u)} q_a - \sum_{a \in \delta^{\text{in}}(u)} q_a = \begin{cases} \ell_u, & u \in V_+, \\ -\ell_u, & u \in V_-, \\ 0, & u \in V_0, \end{cases} \tag{3b}$$

$$\pi_u - \pi_v = \Lambda_a q_a |q_a|, \quad a = (u,v) \in A, \tag{3c}$$

$$0 \le \ell_u \le b_u, \quad u \in V. \tag{3d}$$

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 [24])**.** *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*

$$\varphi_{w_1 w_2}(b) \le \pi^+_{w_1} - \pi^-_{w_2}. \tag{4}$$

For passive tree-shaped or passive single-cycle networks, this characterization can be checked in polynomial time; see [24, 25, 33]. However, the problem of validating a booking on general passive networks is known to be coNP-hard [40].

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^+:

$$V := \{s, v, t\}, \quad A := \{(s, v), (v, t)\},$$

$$\pi^-_s = \pi^+_s = 5, \quad \pi^-_v = 0,\ \pi^+_v = 10, \quad \pi^-_t = 5,\ \pi^+_t = 7,$$

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 $0 \le q_a \le 1$ 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 [36]. 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 $\{(\ell_s, \ell_v, \ell_t) = (x, 0, x) : x \in (0, 0.5]\}$ and the set of feasible nominations $\{(\ell_s, \ell_v, \ell_t) = (x, 0, x) : x \in (0.5, 1]\} \cup \{(0, 0, 0)\}$, 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 [24] 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 [23, 29, 41]. 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 [38, 45] and Section 6 of [20]. 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 Section 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

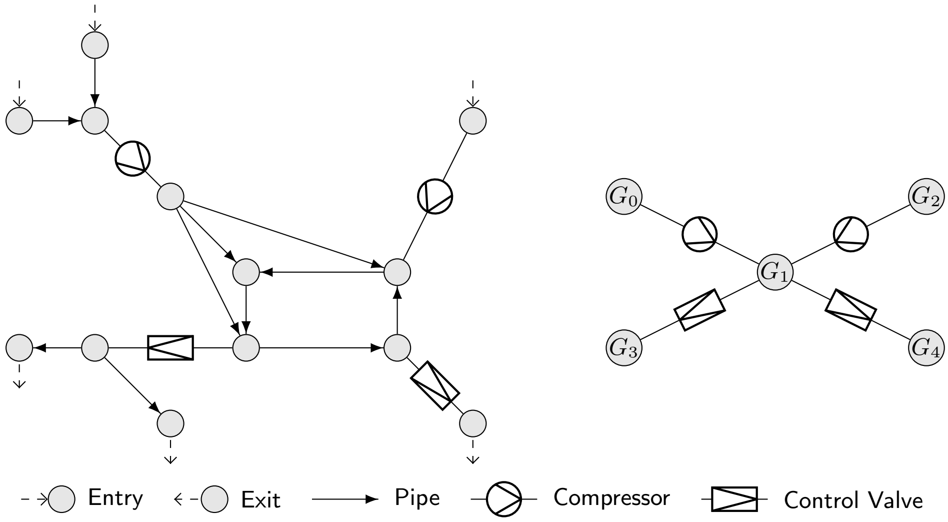

FIGURE 2. Stylized gas network satisfying Assumption 1 (left) and its reduced network (right).

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 [1, 2]. 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 [6, 27, 32] for passive networks.

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 [6, 27]. 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 $A = A_1 \cup A_2 \cup \{a\}$. $\square$

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 [31, 32], we call $\tilde{G}$ the *reduced network*. Figure 2 illustrates a network (left) and its associated reduced network (right).

Using the rationale of [32], 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*

$$\max_{\ell,q,\pi,s} \quad y + z \tag{6a}$$

$$\text{s.t.} \quad (1a), (1b), \tag{6b}$$

$$\ell \in N(b), \tag{6c}$$

$$\pi_u = \pi_v, \quad (u,v) \in A_{\text{act}}, \tag{6d}$$

$$q_a \le m_a(1 - s_a) + M s_a, \quad a \in A_{\text{act}}, \tag{6e}$$

$$s_a \in \{0,1\}, \quad a \in A_{\text{act}}, \tag{6f}$$

$$(\Delta, \tau, y, z) \in \mathcal{R}(\ell, q, \pi, s), \tag{6g}$$

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 [32], 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., [15]. 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

$$\max_{\alpha,\beta,\delta^+,\delta^-} \quad -\sum_{a \in A_{\text{act}}} \Delta_a^+ s_a \beta_a + \sum_{u \in V} \left((\pi_u^- - \pi_u)\delta_u^- - (\pi_u^+ - \pi_u)\delta_u^+\right) \tag{8a}$$

$$\text{s.t.} \quad \sum_{a \in \delta^{\text{out}}(G_j)} \alpha_a - \sum_{a \in \delta^{\text{in}}(G_j)} \alpha_a = \sum_{u \in V(G_j)} (\delta_u^+ - \delta_u^-), \quad G_j \in \mathcal{G}, \tag{8b}$$

$$\alpha_a \le \beta_a, \ \beta_a \ge 0, \quad a \in A_{\text{cm}}, \tag{8c}$$

$$-\alpha_a \le \beta_a, \ \beta_a \ge 0, \quad a \in A_{\text{cv}}, \tag{8d}$$

$$\sum_{u \in V} \delta_u^+ = 1, \ \sum_{u \in V} \delta_u^- = 1, \tag{8e}$$

$$\delta_u^+, \delta_u^- \ge 0, \quad u \in V. \tag{8f}$$

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

$$\max_{\xi} \quad y + z \tag{10}$$
$$\text{s.t.} \quad (6b)\text{–}(6f), \tag{UL}$$
$$(7b)\text{–}(7e), \tag{LLP}$$
$$(8b)\text{–}(8f), \tag{LLD}$$
$$(9),$$

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 [10]. 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

$$\lambda \leq M_{\text{d}} u, \quad c(x) \leq M_{\text{p}}(1 - u),$$

where $u \in \{0, 1\}$ is an auxiliary binary variable and $M_{\text{d}}, M_{\text{p}} \geq 0$ are upper bounds for λ and $c(x)$, respectively. It is shown in [21] 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 $a \in A_{\text{act}}$ 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 $a \in A_{\text{act}}$, 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 $a \in A_{\text{act}}$ the inequality $\Delta_a^+ s_a > 0$ is satisfied. Otherwise, if $\Delta_a^+ s_a = 0$ holds for an arc $a \in A_{\text{act}}$, 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 [22, 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

$$\begin{aligned}
&\tau_i + \varepsilon - \tau_j - \varepsilon + \omega_a \Delta_a = \tau_i - \tau_j + \omega_a \Delta_a = 0, && a = (G_i, G_j) \in A_{\mathrm{act}},\\
&\tau_j + \varepsilon + y - \varepsilon - \tilde{\varepsilon} = \tau_j + y - \tilde{\varepsilon} \geq \pi_u^- - \pi_u - \tilde{\varepsilon}, && u \in V(G_j),\ G_j \in \mathcal{G},\\
&\tau_j + \varepsilon - z - \varepsilon - \tilde{\varepsilon} = \tau_j - z - \tilde{\varepsilon} \leq \pi_u^+ - \pi_u - \tilde{\varepsilon}, && u \in V(G_j),\ G_j \in \mathcal{G}.
\end{aligned}$$

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*

$$\begin{aligned}
0 \leq \pi_u &\leq \sum_{a \in A} \Lambda_a M^2, \quad u \in V,\\
0 \leq \tau_j &\leq \sum_{a \in A_{\mathrm{act}}} \Delta_a^+, \quad G_j \in \mathcal{G},
\end{aligned}$$

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

$$0 \leq \tau_i = \tau_j + \sum_{a \in P(u,v) \cap A_{\mathrm{cm}}} \eta_a(P) \Delta_a - \sum_{a \in P(u,v) \cap A_{\mathrm{cv}}} \eta_a(P) \Delta_a \leq \sum_{a \in A_{\mathrm{act}}} \Delta_a^+. \qquad \square$$

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 Section 5, the bilevel problem (6) can also be reformulated using the lower level's optimal value function; see, e.g., [7]. 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., (LLP) 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

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

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

$$D := \sum_{G_l \in \mathcal{G}_a(G_j)} \sum_{u \in V(G_l)} (\delta_u^+ - \delta_u^-)$$

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 $a = (G_i, G_j) \in A_{\text{act}}^{0,\rightarrow}$,

$$\alpha_a(w_1, w_2) := \begin{cases} -1, & \text{if } G_{j_1} \in \mathcal{G}_a(G_j), G_{j_2} \notin \mathcal{G}_a(G_j),\\ 1, & \text{if } G_{j_1} \notin \mathcal{G}_a(G_j), G_{j_2} \in \mathcal{G}_a(G_j),\\ 0, & \text{otherwise,} \end{cases}$$

and for any $a = (G_i, G_j) \in A_{\text{act}}^{0,\leftarrow}$,

$$\alpha_a(w_1, w_2) := \begin{cases} 1, & \text{if } G_{j_1} \in \mathcal{G}_a(G_i), G_{j_2} \notin \mathcal{G}_a(G_i),\\ -1, & \text{if } G_{j_1} \notin \mathcal{G}_a(G_i), G_{j_2} \in \mathcal{G}_a(G_i),\\ 0, & \text{otherwise.} \end{cases}$$

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 $A_{\text{act}}^{k,\rightarrow}$ and $A_{\text{act}}^{k,\leftarrow}$ can be partitioned similarly. For all $a \in A_{\text{act}}$, we then obtain

$$\alpha_a(w_1, w_2) = \begin{cases} -1, & \text{if } a \in P(G_{j_1}, G_{j_2}) \cap A_{\text{act}}^{j_1,\leftarrow}, \\ 1, & \text{if } a \in P(G_{j_1}, G_{j_2}) \cap A_{\text{act}}^{j_1,\rightarrow}, \\ 0, & \text{otherwise.} \end{cases}$$

Consequently, it also holds

$$\beta_a(w_1, w_2) = \begin{cases} 1, & \text{if } a \in P(G_{j_1}, G_{j_2}) \cap \left(A_{\text{cm}}^{j_1,\rightarrow} \cup A_{\text{cv}}^{j_1,\leftarrow}\right), \\ 0, & \text{otherwise.} \end{cases}$$

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*

$$\max_{\substack{(G_{j_1}, G_{j_2}) \in \mathcal{G}^2, \\ w_1 \in V(G_{j_1}), \\ w_2 \in V(G_{j_2})}} \left\{ \pi_{w_1} - \pi_{w_2} - \left(\pi_{w_1}^+ - \pi_{w_2}^- + \sum_{\substack{a \in P(G_{j_1}, G_{j_2}): \\ a \in A_{\text{cm}}^{j_1,\rightarrow} \cup A_{\text{cv}}^{j_1,\leftarrow}}} \Delta_a^+ s_a \right) \right\}. \tag{14}$$

Similar to the results obtained in [24] 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*

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

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

$$\pi_{w_1} - \pi_{w_2} - \sum_{\substack{a \in P(G_{j_1}, G_{j_2}): \\ a \in A_{\text{cm}}^{j_1,\rightarrow} \cup A_{\text{cv}}^{j_1,\leftarrow}}} \Delta_a^+ s_a \le \pi_{w_1}^+ - \pi_{w_2}^-$$

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.,

$$\pi_{w_1} - \pi_{w_2} - \sum_{\substack{a \in P(G_{j_1}, G_{j_2}): \\ a \in A_{\text{cm}}^{j_1,\rightarrow} \cup A_{\text{cv}}^{j_1,\leftarrow}}} \Delta_a^+ s_a > \pi_{w_1}^+ - \pi_{w_2}^-.$$

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

$$\max_{(G_{j_1},G_{j_2})\in\mathcal{G}^2} \left\{ \begin{aligned} &\max_{w_1\in V(G_{j_1})} \left\{\pi_{w_1} - \pi^+_{w_1}\right\} + \max_{w_2\in V(G_{j_2})} \left\{\pi^-_{w_2} - \pi_{w_2}\right\} \\ &\qquad\qquad - \sum_{\substack{a\in P(G_{j_1},G_{j_2}):\\ a\in A^{j_1,\to}_{\mathrm{cm}}\cup A^{j_1,\leftarrow}_{\mathrm{cv}}}} \Delta^+_a s_a \end{aligned} \right\}. \tag{15}$$

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*

$$\max_{\ell,q,\pi,s} \left\{ \begin{aligned} &\max_{w_1\in V(G_{j_1})} \left\{\pi_{w_1} - \pi^+_{w_1}\right\} + \max_{w_2\in V(G_{j_2})} \left\{\pi^-_{w_2} - \pi_{w_2}\right\} \\ &\qquad\qquad - \sum_{\substack{a\in P(G_{j_1},G_{j_2}):\\ a\in A^{j_1,\to}_{\mathrm{cm}}\cup A^{j_1,\leftarrow}_{\mathrm{cv}}}} \Delta^+_a s_a \quad : \text{(UL)} \end{aligned} \right\}.$$

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 $(G_{j_1},G_{j_2})\in\mathcal{G}^2$ 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

$$\begin{aligned} &P(G_{j_1},G_{j_2})\cap\left(A^{j_1,\to}_{\mathrm{cm}}\cup A^{j_1,\leftarrow}_{\mathrm{cv}}\right) \\ &\subseteq \left(P(G_k,G_{j_1})\cap(A^{k,\leftarrow}_{\mathrm{cm}}\cup A^{k,\to}_{\mathrm{cv}})\right)\cup\left(P(G_k,G_{j_2})\cap(A^{k,\to}_{\mathrm{cm}}\cup A^{k,\leftarrow}_{\mathrm{cv}})\right), \end{aligned} \tag{17}$$

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 $P(G_3,G_2)$.

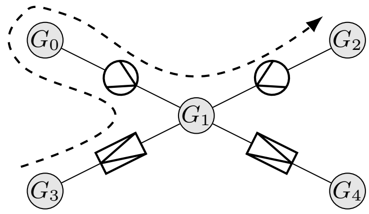

FIGURE 3. Illustration of (17).

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*

$$\begin{aligned}\varphi^k(\ell, q, \pi, s) := & \max_{\substack{G_{j_1} \in \mathcal{G},\\ w_1 \in V(G_{j_1})}} \left\{ \pi_{w_1} - \pi^+_{w_1} - \sum_{\substack{a \in P(G_k, G_{j_1}):\\ a \in A^{k,\leftarrow}_{\mathrm{cm}} \cup A^{k,\rightarrow}_{\mathrm{cv}}}} \Delta^+_a s_a \right\} \\ & + \max_{\substack{G_{j_2} \in \mathcal{G},\\ w_2 \in V(G_{j_2})}} \left\{ \pi^-_{w_2} - \pi_{w_2} - \sum_{\substack{a \in P(G_k, G_{j_2}):\\ a \in A^{k,\rightarrow}_{\mathrm{cm}} \cup A^{k,\leftarrow}_{\mathrm{cv}}}} \Delta^+_a s_a \right\}\end{aligned} \tag{18}$$

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

$$\max_{\substack{(G_{j_1}, G_{j_2}) \in \mathcal{G}^2,\\ w_1 \in V(G_{j_1}),\\ w_2 \in V(G_{j_2})}} \left\{ \pi_{w_1} - \pi^+_{w_1} - \sum_{\substack{a \in P(G_k, G_{j_1}):\\ a \in A^{k,\leftarrow}_{\mathrm{cm}} \cup A^{k,\rightarrow}_{\mathrm{cv}}}} \Delta^+_a s_a + \pi^-_{w_2} - \pi_{w_2} - \sum_{\substack{a \in P(G_k, G_{j_2}):\\ a \in A^{k,\rightarrow}_{\mathrm{cm}} \cup A^{k,\leftarrow}_{\mathrm{cv}}}} \Delta^+_a s_a \right\}.$$

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. □

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,

$$\max_{G_k \in \mathcal{G}} \varphi^k(\ell, q, \pi, s) = \varphi(\ell, q, \pi, s).$$ □

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 $\phi_k(b) \le 0$ 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

$$\vartheta_k^+ = \max_{\substack{G_j \in \mathcal{G},\\ u \in V(G_j)}} \left\{ \pi_u - \pi_u^+ - \sum_{\substack{a \in P(G_k,G_j):\\ a \in A_{\text{cm}}^{k,\leftarrow} \cup A_{\text{cv}}^{k,\rightarrow}}} \Delta_a^+ s_a \right\}, \tag{20a}$$

$$\vartheta_k^- = \max_{\substack{G_j \in \mathcal{G},\\ u \in V(G_j)}} \left\{ \pi_u^- - \pi_u - \sum_{\substack{a \in P(G_k,G_j):\\ a \in A_{\text{cm}}^{k,\rightarrow} \cup A_{\text{cv}}^{k,\leftarrow}}} \Delta_a^+ s_a \right\}. \tag{20b}$$

The optimal value function φ as defined in Theorem 6.7 then is a piecewise-linear function with $|A_{\text{act}}| + 1$ 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 $|A_{\text{act}}| + 1$ 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 $L \le f_i \le U$ holds for every $i \in I$. Then, $g = \max_{i \in I}\{f_i\}$ holds if and only if*

$$f_i \le g \le f_i + (U - L)(1 - u_i), \quad i \in I, \tag{21a}$$

$$\sum_{i \in I} u_i = 1, \;\; u_i \in \{0, 1\}, \quad i \in I. \tag{21b}$$

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 Section 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 Section 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 Section 7.4. We compare the KKT reformulation with the three optimal-value-function reformulations and the three characterizations derived in Section 6. The columns Method and Definition of Table 1 give a short overview regarding the considered methods including their abbreviations used throughout this section.

TABLE 1. Overview of methods and model statistics.

		GasLib-134		GasLib-40	
Method	Definition	Subproblems	Binaries	Subproblems	Binaries
KKT	(10)	1	272	1	90
F-OVF	(12) using (14)	1	17956	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	17956	0	1600	0
R-CHAR	Corollary 6.5	9	162	36	44
S-CHAR	Corollary 6.8	3	268	6	80

7.1. **Data.** Our case study is based on two instances of the GasLib [37] 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 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 μ_1–μ_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 [16]. We performed all computations using the Kaby Lake nodes with 32 GB RAM of the compute cluster [30]. The time limit is 2 h.

In Section 7.3, when treating nonlinear gas physics, we use ANTIGONE 1.1 [28] and BARON 17.4 [39] within GAMS 24.8 [13] to solve the occurring MINLPs. We perform the computations on a single thread and set the optCr parameter in GAMS to 10^{-4}. In Section 7.4, we use Gurobi 9.0.1 [26] 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 Section 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 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., 3.17 s, is faster

Table 2. Results for GasLib-134 and the 2011-11-06 booking in the nonlinear case.

			Time				
Method	Solver	Vio.	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

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 42.64 s, 871.41 s, and 6553.46 s, respectively.

We thus observe a significant increase compared to the running time of 6.93 s 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 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 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

TABLE 3. Results for GasLib-134 and the 2011-11-06 booking in the linear case.

			Time				
Method	Appr.	Vio.	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

individual computations can be done in at most 0.5 s for $c \in \{0.2, 0.4, 0.6, 1.0\}$ and in roughly 1 s 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

TABLE 4. Results for GasLib-40 and the 0–0 booking in the linear case.

			Time				
Method	Appr.	Vio.	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

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 Section 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 [24] 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 Section 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 [24, 33] for tree-shaped and in [25] 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 [5, 35] 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

Table 5. Results for GasLib-134 and the 2012-07-22 booking.

			Time				
Method	Solver	Vio.	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.

			Time				
Method	Solver	Vio.	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

Table 7. Results for GasLib-134 and the 2012-07-22 booking.

			Time				
Method	Appr.	Vio.	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.	Time Min.	Time Med.	Time Max.	Time 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

Table 9. Results for GasLib-40 and the 10–10 booking.

			Time				
Method	Appr.	Vio.	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.	Time Min.	Time Med.	Time Max.	Time 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.

			Time				
Method	Appr.	Vio.	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