Complementarity-Based Nonlinear Programming Techniques for Optimal Mixing in Gas Networks

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Abstract. We consider nonlinear and nonsmooth mixing aspects in gas transport optimization problems. As mixed-integer reformulations of pooling-type mixing models already render small-size instances computationally intractable, we investigate the applicability of smooth nonlinear programming techniques for equivalent complementarity-based reformulations. Based on recent results for remodeling piecewise affine constraints using an inverse parametric quadratic programming approach, we show that classical stationarity concepts are meaningful for the resulting complementarity-based reformulation of the mixing equations. Further, we investigate in a numerical study the performance of this reformulation compared to a more compact complementarity-based one that does not feature such beneficial regularity properties. All computations are performed on publicly available data of real-world size problem instances from steady-state gas transport.

1. Introduction

Pooling problems form a very important class of nonconvex optimization problems. They often appear in practice, e.g., in chemical engineering, and are NP hard to solve in general [1, 40]. We consider a special case of this general problem class from gas transport optimization. Typically, mathematical models from this field combine two aspects: First, they are highly nonlinear due to gas physics and engineering models for machines like compressors. Second, they are discrete in nature due to the control action allowed for certain network elements like compressors or valves. These aspects result in nonconvex mixed-integer nonlinear optimization or feasibility problems (MINLPs) that are hard to solve for instances of real-world size. This field of applied optimization has been highly active in the last years; see, e.g., the recent book [32], the recent survey [43], and the references therein.

Natural gas in transport networks is always a mixture of different gas species. The reason is that different customers inject natural gas to the network that is obtained from different natural resources. These mixtures flow through the network and meet at the network's junctions where they again mix and thus yield new compositions. If one wants to additionally address the physical and chemical effects of different compositions of natural gas one thus has to integrate pooling-type models on top of the already hard MINLPs. In view of the large number of publications on gas transport network optimization in general, mixing effects have been considered less frequently. An early discussion can be found in [55] and more recent modeling approaches with tailored solution methods are presented in [18, 19], which base on the models presented in [51, 52]. The integration of mixing effects is especially important for the practical relevance of gas transport models. Usually these models are formulated in terms of mass flow because it is the most meaningful quantity

Date: January 10, 2019.

2010 *Mathematics Subject Classification.* 90-08, 90C11, 90C33, 90C35, 90C90.

Key words and phrases. Gas transport networks, Mixing, Inverse parametric quadratic programming, Complementarity constraints, MPCC.

in terms of the underlying gas physics. However, accounting in the gas economy is based on heat power and not on mass flows. The relationship between these quantities is given by the calorific value of the gas, which is a composition-specific value that thus has to be tracked through the network by an appropriate mixing model. Similar problems also appear more generally in the context of fluid flow in networks of pipes and canals, if, e.g., water hardness or chemical pollution is to be tracked in fresh or sewage water distribution systems; see [24] for a discussion of these models.

As we will review later in detail, the considered mixing models for gas transport networks are genuinely nonsmooth. To the best of our knowledge, a combination of nonsmooth and integer programming techniques is only beginning to be explored, see, e.g., [7]. Standard smoothing approaches lead to inexact solutions, which may—in particular for the mixing problem under consideration—lead to wrong conclusions concerning feasibility. Since standard models of gas transport networks already involve both nonlinearities and discrete aspects, a rather natural way to reformulate this nonsmoothness exactly is using mixed-integer nonlinear but smooth constraints. However, we show below that the MINLPs, even with integer variables only stemming from the reformulated mixing constraints, are already fully intractable in practice for standard general-purpose solvers. Therefore, alternative reformulations of the mixing equations are of interest. The resulting models should be accessible by smooth nonlinear programming (NLP) techniques whenever integer control variables are fixed or relaxed in order to allow in principle their use within existing MINLP techniques.

In this paper we investigate the use of NLP techniques for complementarity-based reformulations of the mixing constraints. The reformulations lead to so-called mathematical problems with complementarity constraints (MPCCs); see the monograph [37] and the references therein for an in-depth discussion. In general, for the NLP-equivalent of MPCCs, standard constraint qualifications like the linear independence constraint qualification (LICQ) or the Mangasarian–Fromowitz constraint qualification (MFCQ) are typically violated at every feasible point of the problem. However, promising numerical results for applying local NLP solvers to MPCCs have been reported in the literature [12]. A subtle but important drawback of solving MPCCs as NLPs is that it leads to points satisfying MPCC strong stationarity conditions but that these conditions are in general not necessarily satisfied in local optimal points [29].

The main contribution of this paper is to show that the latter issue can be resolved for complementarity-based reformulations of the mixing problem. The result relies on inverse parametric quadratic programming (IPQP), where the evaluation of a continuous and nonsmooth but piecewise affine constraint is replaced by solving a parametric quadratic problem, which can again be replaced by its optimality conditions. The latter step yields an MPCC-type model due to KKT complementarity conditions. This idea has been introduced and analyzed in [26, 27] for problems from the field of optimal control of hybrid systems. We adapt the approach to the mixing problem and compare the numerical performance of such a reformulation with a more compact one lacking a guarantee to provide points satisfying necessary optimality conditions. The computational study is carried out for a significant number of instances from publicly available data of real-world gas transport networks.

While the focus in this study is on the mixing constraints rather than on discrete control aspects, let us also mention that the idea of continuous reformulations of discrete-continuous problems is also frequently used in practice. For instance,

continuous reformulations of MINLPs from process synthesis and chemical engineering are discussed in [33, 34, 53]. The use of MPCC-like reformulations for mixed-integer aspects of gas transport optimization models have been developed by the second author in [44, 49, 50]. Related MPEC models for pipeline operation optimization are also considered in [3]. Moreover, solving MPCCs for computing feasible points of general MINLPs has been recently analyzed in [48]. Finally, the continuous reformulations of the mixing equations obtained here can also be used for non-stationary gas transport problems, where integer controls for valves and compressors may then also be treated using continuous reformulations [22, 23, 25, 45]. We finally note that there is also research on gas transport and gas market problems that use bilevel optimization (see, e.g., [8, 9, 20, 21, 31] and the references therein), which is a field that is closely related to MPCCs. Often, these papers use mixed-integer programming techniques to handle the challenging bi- or multilevel problems. However, the cited references typically use the multilevel structure for economic modeling whereas our complementarity constrained modeling is used for physical aspects of gas flow. As a consequence, our results might also be of use in the applications studied in the above cited papers.

The rest of the paper is structured as follows. In Section 2 we discuss the problem in detail and present all relevant physical and mathematical modeling. Afterward, we present a common mixed-integer reformulation for this problem in Section 3 for which we present numerical results in Section 4. We then derive two different MPCC models of the same problem in Section 5 and discuss the corresponding numerical results in Section 6. The paper closes with some concluding remarks in Section 7.

2. Problem Description

Natural gas plays an increasingly important role as a source of primary energy, especially in many European countries like Germany that use natural gas as some type of bridging energy towards a fully renewable energy sector. Thus, it is an important task to produce, transport, and use natural gas as efficient as possible. We consider the problem of stationary gas transport through gas networks. These networks are highly complex technical entities and their description requires many sophisticated models from engineering, physics, thermodynamics, and mathematics; see, e.g., the book [32] and the survey [43]. Typically, stationary optimization models for gas transport consider gas pressures and mass flows as main physical quantities and formulate the relations between pressures and flows in order to model pressure drop in pipelines, which is the main physical effect in stationary gas transport models. To overcome these pressure losses, compressor stations are incorporated that can increase gas pressure. The energy required for this process is the main cost factor involved in the description of these models and is thus the main aspect to be minimized in the objective function.

However, this physical and technical description does not fully bridge between gas physics and gas economy, in which billing and contracting is based on heating power instead of mass flows. In comparison, this aspect has been addressed in only a few number of publications; see, e.g., [18, 19, 52, 55]. To close the described gap between gas physics and accounting it is required to integrate calorific values and heat power variables into the model. The complicating fact is that different gas sorts with different chemical properties like calorific values then have to be mixed such that the quality parameter of interest can be tracked through the network. This aspect typically leads to pooling-type problems [40] that are known to be extremely challenging NP-hard optimization problems [1].

2.1. General Network Model.

We now describe the problem under consideration and introduce the notation required in the following sections. We consider a gas

transport network modeled by a directed and connected graph $G = (V, A)$. The node set consists of entries V_+, where gas is supplied, of exits V_-, where gas is discharged, and of inner nodes V_0, i.e., $V = V_+ \cup V_- \cup V_0$. The arc set consists of elements representing pipes A_{pi}, compressors A_{cm}, and control valves A_{cm}, i.e., we have $A = A_{\mathrm{pi}} \cup A_{\mathrm{cm}} \cup A_{\mathrm{cm}}$. We are aware of the fact that more holistic models of gas transport networks also incorporate additional devices like valves, resistors, or gas heaters and coolers. However, we refrain from also incorporating these entities in order to focus on the main aspects discussed in this paper.

2.2. **Arcs.** Every arc $a \in A$ is modeled using a gas mass flow variable q_a that is bounded below and above:

$$q_a \in [\underline{q}_a, \bar{q}_a] \quad \text{for all } a \in A. \tag{1}$$

Moreover, we need calorific value variables $H_{\mathrm{c},a}$ for the gas composition flowing through the arc. These variables are bounded below and above by the minimum and maximum calorific values supplied to the network:

$$H_{\mathrm{c},a} \in [\underline{H}_{\mathrm{c},a}, \bar{H}_{\mathrm{c},a}] \quad \text{for all } a \in A. \tag{2}$$

All additional modeling depends on the specific arc type and will be discussed in the following sections.

2.2.1. *Pipes.* Pipes $a = (u, v) \in A$ outnumber all other elements in gas transport networks. Gas physics in cylindrically shaped pipes is described by the Euler equations for compressible fluids. This set of partial differential equations consists of the continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{1}{A}\frac{\partial q}{\partial x} = 0 \tag{3}$$

and the momentum equation

$$\frac{1}{A}\frac{\partial q}{\partial t} + \frac{\partial p}{\partial x} + \frac{1}{A}\frac{\partial (qv)}{\partial x} + g\rho h' + \lambda(q)\frac{|v|v}{2D}\rho = 0. \tag{4}$$

Here, ρ is the gas density, A, D, and $h' \in [-1, 1]$ are the cross-sectional area, the diameter, and the slope of the pipe, p is the gas pressure, and v is the velocity of the gas. Moreover, g describes the gravitational acceleration and $\lambda = \lambda(q)$ models friction at the rough inner pipe walls. Note that we omitted the index a here for better reading. In addition, one has an equation of state for real gas that couples the gas state quantities pressure p, density ρ, and temperature T:

$$p = \rho R_{\mathrm{s}} T z.$$

Here, R_{s} is the specific gas constant and z is the compressibility factor that describes the deviation between ideal and real gas; see, e.g., [15, 51] for more details. We finally remark that we only consider stationary and isothermal regimes, i.e., we neglect all time derivatives in (3) and (4) and further neglect all temperature effects.

A model consisting of the differential equations (3) and (4) would be too complicated to be included into a model that also incorporates mixing effects. This is why we choose to use the well-known finite-dimensional description

$$p_v^2 = \left(p_u^2 - \phi_a(q_a)\frac{e^{S_a} - 1}{S_a}\right) e^{-S_a} \quad \text{for all } a = (u, v) \in A_{\mathrm{pi}} \tag{5}$$

with

$$\Lambda_a = \lambda(q_a)\frac{R_{\mathrm{s}} z_{a,\mathrm{m}} T_{a,\mathrm{m}} L_a}{A_a^2 D_a} = \left(\frac{4}{\pi}\right)^2 \lambda(q_a)\frac{R_{\mathrm{s}} z_{a,\mathrm{m}} T_{a,\mathrm{m}} L_a}{D_a^5}, \quad S_a = \frac{2gh' L_a}{R_{\mathrm{s}} z_{a,\mathrm{m}} T_{a,\mathrm{m}}}.$$

Here, L stands for the length of the pipe and all quantities indexed with "m" represent suitably chosen mean values. The quantity $\phi_a(q_a)$ models a global smooth approximation of the nonsmooth friction term $\Lambda_a |q_a| q_a$. For a derivation of (5) see,

e.g., [15]. The derivation of the global smooth friction term approximation is given in [51].

2.2.2. *Compressor and Control Valves.* Compressors $a = (u, v) \in A_{\mathrm{cm}}$ and control valves $a = (u, v) \in A_{\mathrm{cv}}$ are complex technical devices. Compressors are used to increase the gas pressure in order to transport gas over long distances. In contrast, control valves decrease the gas pressure, which is often required at the transition between large transport pipelines and regional distribution networks. Since our focus is on mixing effects, we refrain from describing and incorporating complex compressor and control valve models including mixed-integer aspects but formulate simple continuous models. The reader is referred to [51] for continuous NLP-type models and to [17], where the authors focus on the discrete aspects of these elements. Instead, we use linear relations between in- and outgoing pressures:

$$p_v = p_u + \Delta_a, \quad \Delta_a \in [\underline{\Delta}_a, \bar{\Delta}_a] \quad \text{for all } a = (u, v) \in A_{\mathrm{cm}}, \tag{6a}$$

$$p_v = p_u - \Delta_a, \quad \Delta_a \in [\underline{\Delta}_a, \bar{\Delta}_a] \quad \text{for all } a = (u, v) \in A_{\mathrm{cv}}. \tag{6b}$$

2.3. **Nodes.** Finally, we describe a general model of nodes. They are modeled by bounded pressure variables

$$p_u \in [\underline{p}_u, \bar{p}_u] \quad \text{for all } u \in V \tag{7}$$

and additional constraints. First of all, mass balance is modeled by classical Kirchhoff-type constraints

$$\sum_{a \in \delta^{\mathrm{out}}(u)} q_a - \sum_{a \in \delta^{\mathrm{in}}(u)} q_a = q_u \quad \text{for all } u \in V, \tag{8}$$

where q_u is the gas mass flow supplied ($q_u > 0$ for all $u \in V_+$) or discharged ($q_u < 0$ for all $u \in V_-$) at node u. If u is an inner node, $u \in V_0$, we set $q_u = 0$. In Constraint (8), we used the standard δ-notation:

$$\delta^{\mathrm{in}}(u) := \{a \in A : \exists v \in V \text{ with } a = (v, u)\},$$
$$\delta^{\mathrm{out}}(u) := \{a \in A : \exists v \in V \text{ with } a = (u, v)\}.$$

Now, we formulate our mixing model, for which we need some more notation. For a node $u \in V$ let

$$\mathcal{I}_u := \{a \in \delta^{\mathrm{in}}(u) : q_a \geq 0\} \cup \{a \in \delta^{\mathrm{out}}(u) : q_a \leq 0\},$$
$$\mathcal{O}_u := \{a \in \delta^{\mathrm{in}}(u) : q_a < 0\} \cup \{a \in \delta^{\mathrm{out}}(u) : q_a > 0\}$$

be the sets of flow-specific ingoing and outgoing arcs, respectively. With this, perfect mixing of calorific values H_{c} at a node u is described by

$$H_{\mathrm{c},u} = \frac{\sum_{a \in \mathcal{I}_u} H_{\mathrm{c},a} \hat{q}_a}{\sum_{a \in \mathcal{I}_u} \hat{q}_a}, \quad \hat{q}_a := \frac{q_a}{m_a} \quad \text{for all } u \in V \setminus V_+, \tag{9}$$

where $H_{\mathrm{c},u}$ models the mixed calorific values at node u. The latter is bounded similarly to the calorific value variables on arcs:

$$H_{\mathrm{c},u} \in [\underline{H}_{\mathrm{c},u}, \bar{H}_{\mathrm{c},u}] \quad \text{for all } u \in V. \tag{10}$$

In the following we assume that all molar masses m_a are equal, which allows to write q_a instead of $\hat{q}_a$ in the mixing equations. At entry nodes, we also have to take into account the calorific value of the supplied gas. Thus, (9) has to be modified to

$$H_{\mathrm{c},u} = \frac{H^{\mathrm{sup}}_{\mathrm{c},u} q_u + \sum_{a \in \mathcal{I}_u} H_{\mathrm{c},a} q_a}{q_u + \sum_{a \in \mathcal{I}_u} q_a} \quad \text{for all } u \in V_+, \tag{11}$$

where the calorific value of the supplied gas at entry node $u \in V_+$ is denoted by $H_{\mathrm{c},u}^{\mathrm{sup}}$. Having these node equations at hand, we finally have to propagate the mixed quantity onto all flow-specific outgoing arcs by

$$H_{\mathrm{c},a} = H_{\mathrm{c},u} \quad \text{for all } u \in V,\ a \in \mathcal{O}_u. \tag{12}$$

Finally, we have contractual constraints at all exit nodes that bound the delivered heat power. Since the latter is simply the product of calorific value and mass flow we obtain the constraints

$$H_{\mathrm{c},u} q_u \in [\underline{P}_u, \bar{P}_u] \quad \text{for all } u \in V_-. \tag{13}$$

2.3.1. *A Nonsmooth Mixing Model.* We now close this section by stating the overall model. Taking all considerations of the previous sections together, we obtain the model

$$\begin{aligned}
\min \quad & \varphi := \sum_{a \in A_{\mathrm{cm}}} \Delta_a && \text{(14a)}\\
\text{s.t.} \quad & \text{variable bounds (1), (2), (7), (10),} && \text{(14b)}\\
& \text{mass balance (8),} && \text{(14c)}\\
& \text{pressure loss in pipes (5),} && \text{(14d)}\\
& \text{compressor and control valve models (6),} && \text{(14e)}\\
& \text{exit heat power bounds (13),} && \text{(14f)}\\
& \text{node mixing equations (9), (11),} && \text{(14g)}\\
& \text{propagation equations (12).} && \text{(14h)}
\end{aligned}$$

The objective function of Model (14) minimizes the overall pressure increase. Of course, more complicated objectives might be possible but we again choose a simple model in order to focus on the mixing aspect of the model.

Model (14) is a nonsmooth and nonconvex optimization problem. Nonconvexity appears in the pressure loss constraints (5) on pipes, in the mixing equations (9) and (11) at nodes, and in the heat power constraints (13) at exits. The nonsmoothness stems from the node mixing equations because the flow-specific sets $\mathcal{I}_u$ and $\mathcal{O}_u$ depend on the problem's solution and, thus, are not known a priori.

3. An MINLP Mixing Model

A straight forward approach to tackle the nonsmoothness of Model (14) is to use an MINLP model for the mixing effects. Remember that the nonsmoothness in Model (14) appears because the sets $\mathcal{I}_u$ and $\mathcal{O}_u$ are not known a priori. However, if we know the flow direction on all arcs of the network, we can formulate the model a priorily. Thus, the main idea of the MINLP model is to introduce a binary variable for every arc of the network that encodes the flow direction on that arc. That is, we introduce the binary variable

$$d_a \in \{0,1\} \quad \text{with} \quad d_a = \begin{cases} 1, & q_a \geq 0, \\ 0, & q_a \leq 0. \end{cases}$$

This can be modeled using the linear constraints

$$(1 - d_a)\underline{q}_a \leq q_a \leq d_a \bar{q}_a \quad \text{for all } a \in A. \tag{15}$$

With this at hand, we can model the splitting of the positive and negative part of every flow via the bilinear formulation

$$\beta_a = d_a q_a, \quad \gamma_a = (d_a - 1) q_a \quad \text{for all } a \in A. \tag{16}$$

That is, we have $q_a = \beta_a - \gamma_a$ with $\beta_a, \gamma_a \geq 0$. On the other hand, it is also possible to formulate a linear model for the splitting of the flow variables. In this formulation, (15) and (16) are replaced by

$$q_a = \beta_a - \gamma, \quad \beta_a \geq 0,\ \gamma_a \geq 0, \tag{17a}$$

$$0 \leq \beta_a \leq d_a \bar{q}_a, \quad 0 \leq \gamma_a \leq (d_a - 1)\underline{q}_a. \tag{17b}$$

The numerical behavior of these two alternative formulations has already been studied for the case of MINLPs from gas transport in [44]. In the next section, we also compare both formulations on our test sets.

With one of the above formulations at hand, we can reformulate the node mixing constraints (9) and (11) as

$$H_{\mathrm{c},u} = \frac{\sum_{a\in\delta^{\mathrm{in}}(u)} \beta_a H_{\mathrm{c},a} + \sum_{a\in\delta^{\mathrm{out}}(u)} \gamma_a H_{\mathrm{c},a}}{\sum_{a\in\delta^{\mathrm{in}}(u)} \beta_a + \sum_{a\in\delta^{\mathrm{out}}(u)} \gamma_a} \quad \text{for all } u \in V \setminus V_+, \tag{18a}$$

$$H_{\mathrm{c},u} = \frac{H^{\mathrm{sup}}_{\mathrm{c},u} q_u + \sum_{a\in\delta^{\mathrm{in}}(u)} \beta_a H_{\mathrm{c},a} + \sum_{a\in\delta^{\mathrm{out}}(u)} \gamma_a H_{\mathrm{c},a}}{q_u + \sum_{a\in\delta^{\mathrm{in}}(u)} \beta_a + \sum_{a\in\delta^{\mathrm{out}}(u)} \gamma_a} \quad \text{for all } u \in V_+. \tag{18b}$$

Multiplication with the denominator reveals that (18) are quadratic constraints.

Finally, the propagation constraints (12) can be reformulated using linear big-M indicator constraints:

$$M(1 - d_a) - (H_{\mathrm{c},a} - H_{\mathrm{c},u}) \geq 0 \quad \text{for all } u \in V,\ a \in \delta^{\mathrm{out}}(u), \tag{19a}$$

$$M(1 - d_a) + (H_{\mathrm{c},a} - H_{\mathrm{c},u}) \geq 0 \quad \text{for all } u \in V,\ a \in \delta^{\mathrm{out}}(u), \tag{19b}$$

$$M d_a - (H_{\mathrm{c},a} - H_{\mathrm{c},u}) \geq 0 \quad \text{for all } u \in V,\ a \in \delta^{\mathrm{in}}(u), \tag{19c}$$

$$M d_a + (H_{\mathrm{c},a} - H_{\mathrm{c},u}) \geq 0 \quad \text{for all } u \in V,\ a \in \delta^{\mathrm{in}}(u). \tag{19d}$$

Instead of these big-M constraints it is also possible to use multiplicative indicator constraints; see [44] for a comparison of different types of indicator constraints in gas transport optimization. However note that $M := \bar{H}_{\mathrm{c},a} - \underline{H}_{\mathrm{c},u}$ is a valid big-M for (19a) and (19c) and $M := \bar{H}_{\mathrm{c},u} - \underline{H}_{\mathrm{c},a}$ is valid for (19b) and (19d). Since these big-M's are quite small in practice, we believe that (19) is the favorable type of indicator constraint in this context.

Thus, we have shown the following result.

Theorem 1. *The solutions of the nonsmooth NLP (14) are in 1:1-correspondence with the solutions of the MINLP*

$$\min \quad \varphi := \sum_{a\in A_{\mathrm{cm}}} \Delta_a \tag{20a}$$

$$\text{s.t.} \quad \textit{variable bounds } (1), (2), (7), (10), \tag{20b}$$

$$\textit{mass balance } (8), \tag{20c}$$

$$\textit{pressure loss in pipes } (5), \tag{20d}$$

$$\textit{compressor and control valve models } (6), \tag{20e}$$

$$\textit{exit heat power bounds } (13), \tag{20f}$$

$$\textit{flow splittings constraints } (15), (16) \textit{ or } (17), \tag{20g}$$

$$\textit{node mixing equations } (18), \tag{20h}$$

$$\textit{propagation equations } (19). \tag{20i}$$

Note that the MINLP (20) has smooth nonlinearities but, of course, this comes at the price of newly introduced binary variables and new linear and nonlinear constraints.

4. Numerical Results for the MINLP Model

In this section we present the numerical results for the MINLP model (20). The section is split up into two parts. First, in Section 4.1 we describe the instances of our test set and discuss our software and hardware setup. Afterward, in Section 4.2 we then present and discuss the numerical results obtained for the MINLP model.

4.1. **Instances and Implementation Details.** For testing and comparing our modeling approaches we use the GasLib, which contains publicly available gas transport network instances; see [30]. We include the following GasLib instances into our test set: the 24-node network GasLib-24, the 40-node network GasLib-40, the 135-node network GasLib-135, and the large 582-node network GasLib-582. For all but the GasLib-582 instance only a single nomination (i.e., a given set of balanced load flows, pressure bounds, quality specifications, etc.) exists. For the GasLib-582 network we randomly choose 50 instances to be included in our test set. The full set of instances is listed in Appendix A. Since our main focus is on mixing models, we modified all supplied calorific values in the GasLib-24, GasLib-40, and GasLib-135 instances using a uniform perturbation between 90 % and 110 % because the original data contains equal values for all entry nodes.

The GasLib instances do not contain any heat power information. Thus, we extend the GasLib instances by choosing the bounds $\underline{P}_u$ and $\bar{P}_u$ (see Constraint (13)) as

$$\bar{P}_u := (1+\alpha)H_{\mathrm{c}}^{\mathrm{m}}\underline{q}_u, \quad \underline{P}_u := (1-\alpha)H_{\mathrm{c}}^{\mathrm{m}}\bar{q}_u \quad \text{for all } u \in V_-$$

with $\alpha \in (0,1)$ and

$$H_{\mathrm{c}}^{\mathrm{m}} := \frac{\sum_{u\in V_+} q_u H_{\mathrm{c},u}^{\mathrm{sup}}}{\sum_{u\in V_+} q_u}.$$

Note that $H_{\mathrm{c}}^{\mathrm{m}}$ is the flow-weighted mean value of the calorific value supplied at all entries. Moreover, among the chosen test sets, the existence of feasible or even optimal solutions is not guaranteed. For computations we choose $\alpha = 0.1$.

All of our models are implemented in GAMS [38] using the C++ framework LaMaTTO++ for modeling and solving mixed-integer nonlinear programming problems on networks [35]. All computations presented below have been carried out on a computer with a 6 core AMD Opteron Processor 2435 processor running at 2.6 GHz and with 64 GB of main memory. All solvers have been applied by using 1 core.

4.2. **Results.** We now present the numerical results for the mixed-integer nonlinear model (20). We first report the numerical results of the global MINLP solvers BARON [46, 54], ANTIGONE [39], and SCIP [16] as well as of the local MINLP solver KNITRO [5] on the small instances GasLib-24, GasLib-40, and GasLib-135. The run times are listed in Table 1. It turns out that these instances are already very hard to solve for the tested solvers. We start with discussing the results for the bilinear flow splitting model (Table 1; top). The smallest instance GasLib-24 can be solved by all solvers but the solution times already differ quite drastically: BARON, KNITRO, and ANTIGONE need less than 1 s (e.g., BARON solves the problem in its presolve stage) whereas SCIP requires 14.1 s. The GasLib-40 instance cannot be solved by SCIP anymore within a time limit of 1 h, whereas BARON and KNITRO solve the problem in a few seconds. ANTIGONE needs more than 30 min to "solve" the problem. However, it wrongly reports that the instance is infeasible. Finally, the GasLib-135 instance cannot be solved by any of the tested solvers within a time limit of 1 h.

Using the linear flow splitting formulation (17) yields comparable results. This has also been reported in [44] for a similar setup of gas transport optimization. It can be seen that the local MINLP solver KNITRO performs better on the linear

TABLE 1. Run times (in s) for the tested MINLP solvers on small networks. For the marked instances, ANTIGONE wrongly reports that the instances are infeasible. Top: Results for the bilinear flow splitting model (15), (16). Bottom: Results for the linear flow splitting model (17).

Run time	BARON	KNITRO	ANTIGONE	SCIP
GasLib-24	0.59	0.91	0.41	14.1
GasLib-40	7.26	15.76	1912.67*	—
GasLib-135	—	—	—	—
GasLib-24	0.38	1.07	0.30	132.40
GasLib-40	29.80	2.52	346.62*	—
GasLib-135	—	2074.10	—	—

formulation and even solves the GasLib-135 to (local) optimality. However, the two global solvers BARON and SCIP need significantly more run time for solving the smaller instances GasLib-24 and GasLib-40. ANTIGONE again delivers the wrong statement of infeasibility for the GasLib-40 network.

Summarizing, it is obvious that the considered class of nonconvex MINLPs is very challenging—also for relatively small networks. This is in line with the recent computational literature on gas network MINLPs [28, 42] and pooling problems in general [40].

We also tested the MINLP formulation for the larger GasLib-582 network. Due to the results on the small networks, we choose to use BARON as a global and KNITRO as a local MINLP solver. Since we are mainly interested in global optimal solutions when solving MINLPs we choose to use the bilinear flow splitting model (15) and (16) because the global solver BARON performs better on this formulation. As expected on the basis of the results on the smaller networks, the global solver BARON was not able to solve any of the 50 tested instances within the time limit of 1 h. The local solver KNITRO was a little bit more successful. It can solve 3 instances to (local) optimality and 12 more to feasibility. This corresponds to 30 % of the instances that can be solved at least to feasibility. The remaining 35 instances were wrongly detected to be (locally) infeasible (32 instances) or the solver hit the time limit (for 3 instances). Note finally that all 12 instances that are solved to feasibility also reached the time limit, i.e., KNITRO is able to find a feasible solution within 1 h but is not able to prove (local) optimality. The three instances solved to optimality required 100, 191, and 135 s.

Altogether the results for the MINLP formulation of the mixing model are not convincing. It is almost impossible to solve reasonably sized instances to global optimality and also local optimality could only be computed for 6 % of the GasLib-582 instances. This legitimates the study of local approaches for alternative continuous formulations of the problem.

5. Complementarity-Based Reformulations

The nonsmooth constraints of Model (14) can also be tackled using complementarity constraints. This can be done in several ways and our focus will be on whether one of these ways is advantageously. In view of regularity conditions, we say that a set of constraints is *mild* if any local minimum of a given and sufficiently smooth cost function subject to these constraints satisfies the classical KKT conditions. It is well-known that complementarity constraints are in general not mild because they typically violate standard constraint qualifications. The main result in this

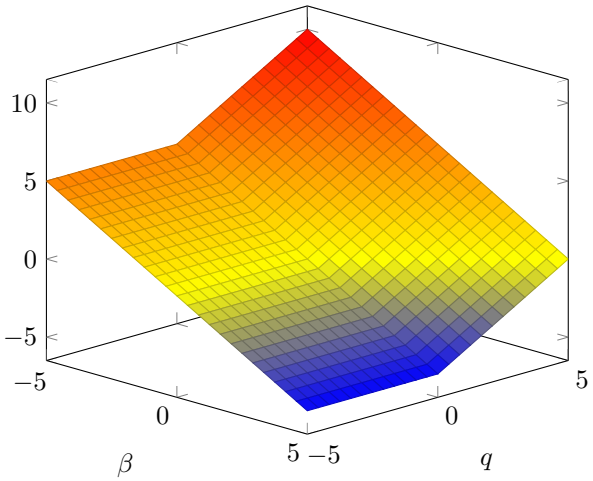

FIGURE 1. The nonsmooth function $f(z) = \max\{0, q\} - \beta$

section is that the mixing model admits a reformulation with mild complementarity constraints.

Recalling that the problem with Model (14) are the sets $\mathcal{I}_u$ and $\mathcal{O}_u$ for each node $u \in V$ (because these sets are not known a priori), we replace the sets $\mathcal{I}_u$ and $\mathcal{O}_u$ for each node as in the MINLP formulation with the a priorily given sets $\delta^{\text{in}}(u)$ and $\delta^{\text{out}}(u)$ for every u. For this, we use nonsmooth max-constraints that depend on the flow directions instead of introducing binary variables.

To this end consider the constraint

$$f(z_a) = \max\{0, q_a\} - \beta_a = 0, \quad z_a = (q_a, \beta_a)^\top, \tag{21}$$

i.e., β_a models the positive part of the mass flow q_a as it was also the case for the mixed-integer model (16); see also Figure 1. Note that

$$\max\{0, -q_a\} = \beta_a - q_a$$

holds. That is, $\beta_a - q_a$ takes to role of γ_a in the MINLP model (16). This allows us to rewrite the mixing models (9) and (11) as

$$H_{c,u} = \frac{\sum_{a\in\delta^{\text{in}}(u)} \beta_a H_{c,a} + \sum_{a\in\delta^{\text{out}}(u)} (\beta_a - q_a) H_{c,a}}{\sum_{a\in\delta^{\text{in}}(u)} \beta_a + \sum_{a\in\delta^{\text{out}}(u)} (\beta_a - q_a)} \tag{22a}$$

for all $u \in V \setminus V_+$ and

$$H_{c,u} = \frac{H_{c,u}^{\text{sup}} q_u + \sum_{a\in\delta^{\text{in}}(u)} \beta_a H_{c,a} + \sum_{a\in\delta^{\text{out}}(u)} (\beta_a - q_a) H_{c,a}}{q_u + \sum_{a\in\delta^{\text{in}}(u)} \beta_a + \sum_{a\in\delta^{\text{out}}(u)} (\beta_a - q_a)} \tag{22b}$$

for all $u \in V_+$ and the propagation of the mixed node quantities as

$$\beta_a (H_{c,a} - H_{c,u}) = 0 \quad \text{for all } u \in V,\ a \in \delta^{\text{out}}(u), \tag{23a}$$

$$(\beta_a - q_a)(H_{c,a} - H_{c,u}) = 0 \quad \text{for all } u \in V,\ a \in \delta^{\text{in}}(u). \tag{23b}$$

We now derive complementarity-based reformulations of the nonsmooth constraint (21). For reasons of better reading we drop the arc index a in the following before returning to the full model again at the end of the section. Observe that the function $f\colon \mathbb{R}^2 \to \mathbb{R}$ used in (21) is continuous, convex, and piecewise affine (PWA). Partitioning

$$\mathbb{R}^2 = \Omega_1 \cup \Omega_2$$

with

$$\Omega_1 = (-\infty, 0] \times \mathbb{R}, \quad \Omega_2 = [0, +\infty) \times \mathbb{R}$$

yields

$$f\restriction_{\Omega_1} = -\beta, \quad f\restriction_{\Omega_2} = q - \beta.$$

The constraint $f(z) = 0$ can directly be reformulated as a complementarity constraint.

Lemma 1. *For all $\beta, q \in \mathbb{R}$ we have*

$$f(z) = 0 \iff \beta = \max\{0, q\} \tag{24}$$

if and only if

$$\beta \geq 0, \quad \beta - q \geq 0, \tag{25a}$$

$$\beta(\beta - q) = 0. \tag{25b}$$

Proof. (24) $\Longrightarrow$ (25): If $q < 0$, then $\beta = 0$ and it is easy to see that (q, β) solves (25). If $q \geq 0$, then $\beta = q$ and again it is easy to see that (q, β) solves (25).

(25) $\Longrightarrow$ (24): If $q \leq 0$ and $\beta > 0$, then (25b) implies $\beta - q = 0$, a contradiction. If $q \leq 0$ and $\beta = 0$, then (q, β) solves (25) and it holds $\beta = 0 = \max\{0, q\}$. If $q \geq 0$ and $\beta > 0$, then (25b) implies $q - \beta = 0$, hence $q = \beta = \max\{0, q\}$. If $q \geq 0$ and $\beta = 0$, then (25a) implies $q \leq 0$, hence $q = 0$ and it holds $\beta = 0 = \max\{0, q\}$. □

Similar reformulations can also be found in the MacMPEC library of MPEC problems [36]. It is known that the formulation (25b) using an equality constraint may be numerically disadvantageous and that the equivalent formulation $\beta(\beta - q) \leq 0$ using an inequality leads to more stable results; see, e.g., [13]. Thus, in the following we always use the inequality constrained version.

The set of constraints (25) are rather simple but not mild; see, e.g., [37]. Typically, alternative constraint qualifications and stationarity concepts are used (see, e.g., [47]) or tailored regularization techniques are applied; see, e.g., [29]. The focus of this paper, however, is on exact complementarity-based reformulations without any further regularization such that results like Theorem 1 can also be shown for the obtained MPCC-type models. Fortunately, alternative complementarity reformulations are possible. A systematic way to obtain such reformulations is inverse parametric quadratic optimization. The general idea is to write a piecewise affine constraint itself as a solution of an appropriate parametric optimization problem and to make use of its optimality conditions instead of the original constraint. Interestingly, this can be done exactly and leads to mild constraints similarly as in the case of hybrid dynamical systems [26, 27].

Lemma 2 ([27, Lemma 9])**.** *Let $f\colon \mathbb{R}^m \to \mathbb{R}^n$ be a continuous PWA function such that every component $f_i\colon \mathbb{R}^m \to \mathbb{R}$ is convex for all $i \in \{1, \dots, n\}$. Then*

$$f(z) = \operatorname*{argmin}_{\xi \in \mathbb{R}^n} \left\{ \frac{1}{2} \|\xi - \bar{f}(z)\|_Q^2 \ : \ \xi \geq f(z) \right\} \tag{26}$$

for any positive definite $n \times n$ diagonal matrix Q and any affine function $\bar{f}\colon \mathbb{R}^m \to \mathbb{R}^n$ with

$$\bar{f}(z) \leq f(z) \quad \text{for all } z \in \mathbb{R}^m. \tag{27}$$

We can apply Lemma 2 to the convex PWA function $f(z)$ of Constraint (21) with $m = 2$ and $n = 1$ choosing $Q = 1$ and $\bar{f}(z) = -z_2 - \eta$ for arbitrary $\eta > 0$. Then we have

$$\bar{f}(z) = -z_2 - \eta = -\beta - \eta < \max\{0, q\} - \beta = f(z). \tag{28}$$

In particular, (27) holds strictly. Hence, using the variables $z = (q, \beta)$ and ignoring constant terms in the cost function in (26), we obtain

$$f(q,\beta) = \operatorname*{argmin}_{\xi\in\mathbb{R}} \left\{ \frac{1}{2}\xi^2 + (\beta+\eta)\xi \,:\, \xi \geq -\beta, \xi \geq q-\beta \right\}. \tag{29}$$

Using that Slater's constraint qualification is satisfied for each fixed q and β (i.e., there exists a ξ with $\xi > -\beta$ and $\xi > q - \beta$), the unique solution of the quadratic program in (29) is characterized by its KKT conditions

$$\begin{aligned} \xi + \beta + \eta - \lambda_1 - \lambda_2 &= 0, \\ \beta + \xi \geq 0, \quad \beta + \xi - q &\geq 0, \\ \lambda_1, \lambda_2 &\geq 0, \\ \lambda_1(\beta+\xi) = 0, \quad \lambda_2(\beta+\xi-q) &= 0. \end{aligned} \tag{30}$$

Using that $f(z) = 0$ yields $\xi = 0$, we obtain another complementarity reformulation.

Lemma 3. *For all $\beta, q \in \mathbb{R}$ we have*

$$f(z) = 0 \iff \beta = \max\{0, q\} \tag{31}$$

if and only if

$$\beta + \eta - \lambda_1 - \lambda_2 = 0, \tag{32a}$$
$$\beta \geq 0, \quad \beta - q \geq 0, \tag{32b}$$
$$\lambda_1, \lambda_2 \geq 0, \tag{32c}$$
$$\lambda_1\beta = 0, \quad \lambda_2(\beta - q) = 0. \tag{32d}$$

As discussed after Lemma 1, the equality constraints in (32d) can be equivalently replaced by the corresponding inequality constrained versions

$$\lambda_1\beta \leq 0, \quad \lambda_2(\beta - q) \leq 0$$

that we use in the following.

One can easily verify that MPCC-LICQ (see, e.g., [14, 29] for a definition) holds for both constraint sets (25) and (32). Moreover, for the latter it is possible to show the following additional regularity property, for which we make use of the Abadie constraint qualification (ACQ), which is defined to be satisfied at a feasible point x^* if the tangential cone $T_\Omega(x^*)$ coincides with the linearization cone $\mathcal{L}(x^*)$. The definitions of standard constraint qualifications as well as the mentioned cones can be found in, e.g., [4, 41].

Proposition 1. *For any sufficiently smooth cost function, the set of constraints given by (32) is mild and the ACQ is satisfied at every point that is feasible for (32).*

Proof. Noting (28), the proposition follows from the proofs of Theorem 1 and Theorem 5 in [27] because f is a particular instance of a continuous PWA function. □

Corollary 1. *Under the assumptions of Proposition 1, the set of constraints*

$$\beta + \eta - \lambda_1 - \lambda_2 = 0, \tag{33a}$$
$$\beta \geq 0, \quad \beta - q \geq 0, \tag{33b}$$
$$\lambda_1, \lambda_2 \geq 0, \tag{33c}$$
$$\lambda_1\beta \leq 0, \quad \lambda_2(\beta - q) \leq 0. \tag{33d}$$

is mild.

Proof. From Proposition 1 we know that the ACQ is satisfied for every feasible point of (32). The difference between (32) and (33) is that we replaced the equality constraints in (32d) with inequalities. The mildness of (32) implies that the corresponding tangential cone $T_\Omega^=(x^*)$ and the linearization cone $\mathcal{L}^=(x^*)$ coincide, i.e., $T_\Omega^=(x^*) = \mathcal{L}^=(x^*)$ holds. Moreover, the tangential cone corresponding to formulation (32) is equal to the tangential cone $T_\Omega^\leq(x^*)$ for the formulation (33) because tangential cones only depend on the geometry of the feasible sets, which are the same for both formulations. That is, we have $T_\Omega^=(x^*) = T_\Omega^\leq(x^*)$. An easy computation also reveals that $\mathcal{L}^=(x^*) = \mathcal{L}^\leq(x^*)$ holds, i.e., also the linearization cones of (32) and (33) are the same. Thus, we have

$$\mathcal{L}^\leq(x^*) = \mathcal{L}^=(x^*) = T_\Omega^=(x^*) = T_\Omega^\leq(x^*).$$

Thus, the inequality constrained formulation is mild as well. □

As we already pointed out, KKT conditions typically cannot be used directly as a proper stationarity concept for MPCCs. Since almost all NLP solvers rely on this concept, they may (despite convergence issues) fail to provide local minima; see, e.g., [2, 6, 11]. The main implication of Proposition 1 is that this failure of the KKT stationarity concept does not apply in the case of the constraint set (32), which legitimates the application of standard NLP solvers.

Note further that the above results extend more generally to continuous PWA functions using DC decompositions [26, 27].

Returning to the full gas network model again, applying Lemma 3 to the constraints $f(z_a) = 0$ for all $a \in A$, we obtain the complementarity conditions

$$\begin{aligned} \beta_a \geq 0, \quad \beta_a - q_a \geq 0, \\ \beta_a(\beta_a - q_a) \leq 0 \end{aligned} \tag{34}$$

from Lemma 1 or the complementarity conditions

$$\begin{aligned} \beta_a + \eta - \lambda_{a_1} - \lambda_{a_2} = 0, \\ \beta_a \geq 0, \quad \beta_a - q_a \geq 0, \\ \lambda_{a_1}, \lambda_{a_2} \geq 0, \\ \lambda_{a_1}\beta_a \leq 0, \quad \lambda_{a_2}(\beta_a - q_a) \leq 0 \end{aligned} \tag{35}$$

from Corollary 1. With this we have shown the following result.

Theorem 2. *The solutions of the nonsmooth NLP (14) are in 1:1-correspondence with the solutions of the MPCC*

$$\begin{aligned} \min \quad & \varphi := \sum_{a \in A_{\mathrm{cm}}} \Delta_a && \text{(36a)} \\ \text{s.t.} \quad & \textit{variable bounds } (1), (2), (7), (10), && \text{(36b)} \\ & \textit{mass balance } (8), && \text{(36c)} \\ & \textit{pressure loss in pipes } (5), && \text{(36d)} \\ & \textit{compressor and control valve models } (6), && \text{(36e)} \\ & \textit{exit heat power bounds } (13), && \text{(36f)} \\ & \textit{node mixing equations } (22), && \text{(36g)} \\ & \textit{propagation equations } (23), && \text{(36h)} \\ & \textit{complementarity constraints } (34) \textit{ or } (35). && \text{(36i)} \end{aligned}$$

Note that, in contrast to Problem (20), (36) does not contain any integer variables. Furthermore, note that instances of both MPCCs with (34) or (35) in (36) will typically violate constraint qualifications such as LICQ or MFCQ. However,

TABLE 2. Run times (in s) for the tested NLP solvers on small networks. Complementarity constraints modeled as equalities (top) and as inequalities (bottom)

	CONOPT4		SNOPT		KNITRO		Ipopt	
	Direct	IPQP	Direct	IPQP	Direct	IPQP	Direct	IPQP
GasLib-24	0.14	0.10	0.08	0.09	0.13	0.15	—	—
GasLib-40	0.50	—	0.28	4.22	33.04	—	—	—
GasLib-135	—	—	16.69*	—	—	—	—	—
GasLib-24	0.14	0.10	0.091	0.10	0.15	0.15	2.21	2.10
GasLib-40	0.47	0.67	0.396	2.85	4.75	2.11	3.12	11.97*
GasLib-135	—	—	18.435	3.03	25.62	37.51	5.88*	138.84*

Proposition 1 shows that using (35) in (36) may be beneficial for an NLP solver in terms of constraint regularity.

6. Numerical Results for the Complementarity-Based Models

In this section we present the numerical results for the two different versions of the MPCC-type model (36) that differ depending on whether the complementarity-based constraints of Lemma 1 (called MPCC-Direct in the following) or Lemma 3 (called MPCC-IPQP in the following) are used. The theoretical advantages and drawbacks of both variants are easy to see: The variant MPCC-Direct is smaller in terms of the number of variables as well as in the number of linear and complementarity constraints. On the other hand, the variant MPCC-IPQP uses mild complementarity constraints and thus has favorable regularity properties. The purpose of this section is to analyze how these two formulation behave computationally.

All complementarity constraints are used as stated in (34) and (35), respectively, without any further regularization or relaxation. Note that this yields a violation of classical constraint qualifications like LICQ or MFCQ and that, thus, the convergence theory of typical NLP solvers does not formally hold. Nevertheless, at least for the mild reformulation, the solutions are meaningful if the solvers terminate. For our study, we consider the four local NLP solvers CONOPT4, SNOPT, KNITRO, and Ipopt. The software and hardware setup is the same as described in Section 4 except for the significantly decreased time limit of 10 min. Our preliminary numerical tests revealed that time limits larger than 10 min do not change the results qualitatively. Moreover, we choose $\eta = 10^{-6}$; see (28).

We start by discussing the numerical results obtained for the small networks that we also considered for the MINLP formulations in Section 4; see Table 1. The results are given Table 2. We applied all NLP solvers both for the MPCC-Direct and the MPCC-IPQP formulation as well as for the equality and inequality constrained formulation. The first insight is that the inequality constrained formulation performs better; both in terms of running times and in terms of the overall solved instances. Regarding the failures of Ipopt we need to remark that this solver never starts to solve an equality constrained formulation because it complains about a larger number of equality constraints than variables.

In what follows, we focus on the inequality constrained modeling. SNOPT, KNITRO, and Ipopt solve all instances using MPCC-Direct and the MPCC-IPQP formulation. On the other hand, CONOPT4 is very fast if it solves a given instance at all. Finally, we consider the solutions provided by the solvers. Since they all are local solvers that we apply to a nonconvex problem, we might obtain local

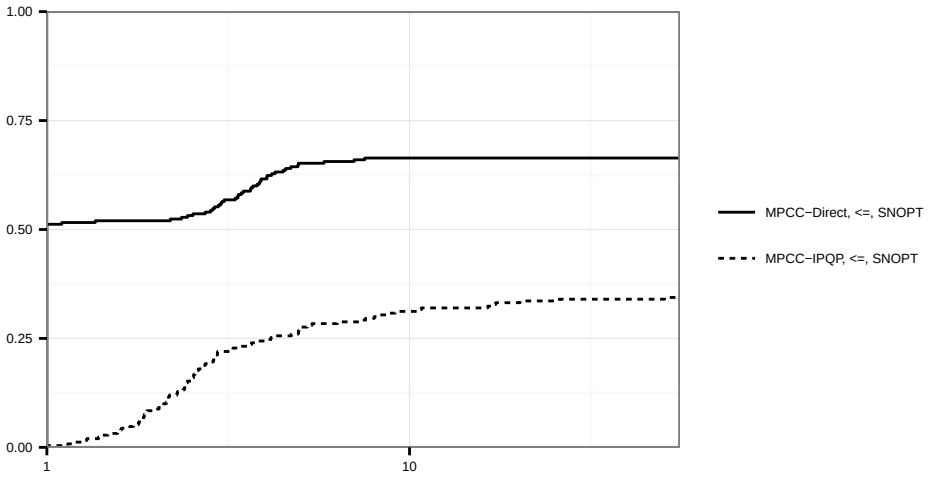

FIGURE 2. Log-scaled performance profile of SNOPT applied to the MPCC-Direct and MPCC-IPQP models on 250 randomly chosen instances of the GasLib-582 network

optima. Fortunately, in almost all cases the local solvers provide the global optimal solutions. Only those instances that are marked with an asterisk are solved to a local optimal point that is not the global optimum, which is particularly the case for Ipopt. Moreover, we see that the success depends both on the formulation and the solver: For the largest instance GasLib-135, SNOPT is significantly faster when applied to the MPCC-IPQP formulation, whereas KNITRO is faster when applied to the smaller MPCC-Direct model. In summary, the MPCC models significantly outperform the MINLP models on these networks. They can be solved for many more instances and, in most of the cases, deliver globally optimal solutions.

In order to further test the MPCC formulations we use 250 randomly chosen nominations for the GasLib-582 network (see Section 4.1 for general information on GasLib and Appendix A for the full list of all 250 nominations). For these larger instances, both KNITRO and Ipopt generally have severe convergence issues. We therefore discard their very poor results in the comparison for these larger instances. For the two remaining solvers SNOPT and CONOPT4, we can then separately compare both model variants by using performance profiles as proposed in [10] with run times as the performance measure.

We start by discussing the results for SNOPT. The corresponding performance profile is given in Figure 2. SNOPT seems to cope well with the complementarity-constrained models at hand. In particular, it does not benefit from the gain of regularity of the MPCC-IPQP model, for which only 86 instances (34.4 %) are solved. In contrast, the more compact MPCC-Direct is solved 166 times (66.4 %). Moreover, the latter model variant is solved faster than the IPQP-based model for slightly more than 50 % of the instances. Thus, SNOPT seems to benefit from the more compact model with less complementarity constraints more than from constraint regularity. This is in line with the observations reported in [14]. The solver SNOPT implements an "elastic mode" that uses an automatically chosen relaxation of inconsistent QP subproblems. As our results indicate, this strategy of SNOPT seems to work better for the more compact MPCC model. However, in this comparison, one has to keep in mind that solutions of MPCC-Direct are not guaranteed to satisfy necessary optimality conditions while solutions of MPCC-IPQP do; see Corollary 1.

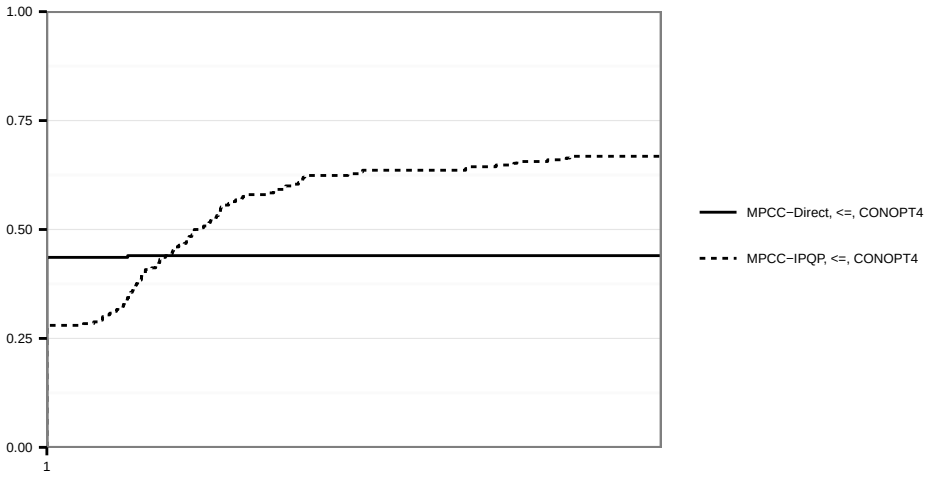

FIGURE 3. Log-scaled performance profile of CONOPT4 applied to the MPCC-Direct and MPCC-IPQP models on 250 randomly chosen instances of the GasLib-582 network

TABLE 3. Number of solved instances (out of 250) and statistics for the solution times (always taken only for all instances solved to optimality)

	SNOPT		CONOPT4	
	Direct	IPQP	Direct	IPQP
# solved	166	86	110	167
Minimum	2.780	8.779	3.133	5.025
1st Quantile	4.698	12.250	4.257	5.719
Median	5.602	14.210	4.518	6.259
Mean	6.246	26.540	4.687	7.263
3rd Quantile	6.836	24.060	5.035	7.274
Maximum	76.440	399.300	9.139	16.330

The situation changes significantly when we turn to the numerical results obtained by CONOPT4; see Figure 3. We again see that the more compact model formulation is solved faster almost always if it is solved at all (see the almost horizontal line in Figure 3). However, the gain of mildness of variant MPCC-IPQP yields a significantly more reliable solution approach: 66.8 % of the instances (167 of 250) are solved—in contrast to only 44 % (110 of 250) for the MPCC-Direct model.

In summary, we see that the relevance of mildness strongly depends on the chosen solver technology and thus the choice of the specific solver and the model should be done carefully and in combination of each other. Moreover, model size and mildness seem to be competing measures. This can also be seen in Table 3: For both solvers the MPCC-Direct model is solved faster than the MPCC-IPQP variant. Thus, it is an open question whether there exist formulations that are both mild and compact.

Finally, let us compare the MPCC-based numerical results with those of the MINLP model. For the latter, it is only possible to solve the much smaller GasLib-135 instance to local optimality within the time limit of 1 h and almost no instances can be solved for the GasLib-582 network. In contrast, using CONOPT4 and the MPCC-IPQP model variant we can solve more than 66 % of all instances within less

than 10 s. Obviously, this comes at the price of local solutions but the enormous difference in success rates between the MINLP and MPCC models indicates that complementarity-based models are clearly favorable.

7. Conclusion

In this paper we investigated mixing models for different gas compositions in gas transport networks. The focus is on exact reformulations of nonsmooth aspects of the mixing equations. This especially means that we neither apply smoothings of nonsmooth aspects nor regularizations of the considered MPCCs. It turned out that classical MINLP formulations become intractable already on quite small networks. Purely continuous reformulations of MPCC-type significantly outperform the discrete-continuous model variants. The comparison between the different MPCC models shows that performance and reliability strongly depends on the chosen solver.

Since it turned out that MPCC model size and constraint regularity are competing aspects, the main question for future research is to determine if both compact and mild complementarity-based models exist.

Acknowledgements

This research has been performed as part of the Energie Campus Nürnberg and is supported by funding of the Bavarian State Government and by the Emerging Field Initiative (EFI) of the Friedrich-Alexander-Universität Erlangen-Nürnberg through the project "Sustainable Business Models in Energy Markets". The authors acknowledge funding through the DFG Transregio 154, subprojects A03, A05, and B08. Finally, we thank Sebastian Peuker for his support with implementing the models.

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Appendix A. GasLib-582 Test Set

Table 4. 50 randomly chosen GasLib-582 instances

nomination_cold_95_									
1202	1317	1361	1432	1689	1948	1974	2049	2161	2205
2329	2628	3146	3285	421	596	634	740		
nomination_cool_95_									
1036	1398	1776	2301	2394	2535	2794	3121	3594	524
710	720								
nomination_freezing_95_									
2302	2587	2877	3105	3320	3408	3850	4199	495	
nomination_mild_95_									
1070	175	1934	1964	2594	3499	3669	3766	805	92
nomination_warm_95_									
3536									

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TABLE 5. 250 randomly chosen GasLib-582 instances

nomination_cold_95_									
1277	1278	1300	1315	1426	1527	1572	162	1662	1722
176	1828	1834	1835	1878	1904	2071	2102	2123	2149
2340	2423	2436	2446	2519	2543	2681	2720	2722	2799
2820	2855	2856	2998	301	3082	3136	3162	3246	3335
3338	3495	3514	3598	3739	3807	3813	3824	3894	395
4000	4054	4155	480	503	542	573	680	722	868
873	905	906	914						
nomination_cool_95_									
1010	1012	1036	109	1166	1294	1337	1365	1394	1530
1622	1641	1654	1744	1779	1852	1886	1987	2040	2064
2078	2084	2150	2217	2320	233	2426	2597	2608	2656
2680	2797	285	2867	287	2954	2992	2999	3013	3079
3154	3181	3209	3269	3283	3322	3324	3492	3518	3667
3753	3788	3808	3854	3869	3	4004	4067	411	4179
456	498	514	685	699	813	847	951	988	
nomination_freezing_95_									
1205	1268	129	1320	1583	1712	1821	1844	2183	2236
2242	2420	2457	2491	2536	2545	2664	2710	2719	2800
2853	2890	3122	3189	3311	3320	3345	3392	3398	3410
3414	3465	354	3648	3657	3732	402	4035	4040	4061
4113	440	458	647	836	867	870			
nomination_mild_95_									
1142	1159	1198	1218	140	1454	1455	1817	1866	1867
1945	1961	1969	2030	2081	2134	2235	2265	2282	241
246	2661	2727	2732	2930	3230	3432	3436	3480	3553
369	3701	3838	3844	3999	405	4110	4169	4170	605
648	70	837	931	949	956				
nomination_warm_95_									
1062	1112	1146	124	1353	1594	1716	1747	181	2246
2610	2666	2899	3021	324	3331	3366	338	357	3725
4160	597	638	848						