Improving relaxations for potential-driven network flow problems via acyclic flow orientations*

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Abstract

The class of potential-driven network flow problems provides important models for a range of infrastructure networks. For real-world applications, they need to be combined with integer models for switching certain network elements, giving rise to hard-to-solve MINLPs. We observe that on large-scale real-world *meshed* networks the usually employed relaxations are rather weak due to cycles in the network. We propose *acyclic flow orientations* as a combinatorial relaxation of feasible solutions of potential-driven flow problems and show how they can be used to strengthen existing relaxations. First computational results indicate that the strengthend model is much tighter than the original relaxation, thus promising a computational advantage.

Network operators for utility and infrastructure networks face difficult planning and operational problems [4, 11, 20, 10]. Due to regulation and increasing cost pressure, but also due to the availability of powerful solvers, modern optimization methods are more and more applied to reduce cost and to improve the quality of planning and operation. The complexity of the considered optimization problems increases for several reasons, for instance because geographically bigger networks are considered or the detail level is increased. For instance, realistic network models for parts of the German gas network have more than 4000 nodes and almost 4500 arcs [26]. For networks of this size, providing globally optimal solutions or at least good bounds for assessing solution quality is still a big challenge [10].

A key submodel for infrastructure networks for fluids, e.g., water and gas [23, 6, 11], is the so-called *potential-driven nonlinear network flow problem.* This problem features a so-called *potential* π_u for each node $u \in V$, and the flow q_a of an arc $a \in A$ is related to the difference of the potential of its end nodes via an arc-specific *potential loss function* ϕ_a. Formally, the potential-driven network flow problem for a digraph $D = (V, A)$, supply vector q^{nom}, and bounds on the

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flow q_a and potential π_u is given by

$$
\begin{aligned}
\min \quad & c^T(q, \pi, s) && && \text{(1a)}\\
q_v^{\text{nom}} + \sum_{a=uv\in A} q_a - \sum_{a=vu\in A} q_a &= 0 && \text{for all } v \in V, && \text{(1b)}\\
\pi_u - \pi_v &= \phi_a(q_a) && \text{for all } a \in A, && \text{(1c)}\\
\underline{q}_a \le q_a &\le \overline{q}_a && \text{for all } a \in A, && \text{(1d)}\\
\underline{\pi}_u \le \pi_u &\le \overline{\pi}_u && \text{for all } u \in V. && \text{(1e)}
\end{aligned}
$$

An important property of this model is that the flow is always directed from higher to lower potential, i.e., the potentials induce an acylic orientation of the arcs. In other words: The network arising from a *feasible* flow by orienting each network arc in the direction of the flow over this arc contains no directed cycle.

This property is only implicit in the model for potential-driven network flows, i.e., it is not represented by an explicit constraint, but follows from the interplay of flow conservation and potential loss along an arc. Therefore, it is not reflected in the relaxations used to solve these nonlinear noncovex optimization problems. We discuss this in detail in Section 1.

Our contribution This paper proposes to use the discrete structure arising from the combination of flow conservation and an acyclicity requirement for the flow to improve the relaxations used to solve MINLPs arising from potential-driven network flow problems to global optimality. To this end, we introduce a combinatorial abstraction of feasible flows we call *acyclic flow orientation*. As real networks contain additional network elements that do not necessarily fit the potential-driven network flow framework, we consider a generic MINLP featuring the potential-driven network flow problem as a submodel. Moreover, we consider not only fixed demand vectors, but intervals for the demand at each source/sink. This is useful for situations where the demand is not fully fixed, e.g., due to mixing of gas qualities [9]. Moreover, this may be applied to analyze the difference in flow directions if large classes of demand vectors are possible [18].

Related work Potential-driven network flow problems have been considered at least since the 1970s [21, 5] and are relevant for a variety of applications areas [16]. Although *pure* potential-driven network flow problems (1) are nonconvex NLPs, their special structure enables the development of efficient solution techniques [5]. For network design problems, binary variables for enabling/disabling network elements are introduced, yielding MINLPs that are NP-hard [14] and significantly harder to solve in practice [23, 19]. The same holds when the problem is extended by models for further (switchable) network elements to model network operation in detail [22, 20, 10].

For the case of the potential network flow problem (1) with potential loss function $\phi_a(q_a) = c_a q_a |q_a|$, knowing the flow directions for all arcs enables the use of algebraic methods to e.g., solve certain stochastic optimization variants of the problem [12, 13]. Enumerating all acyclic flow orientations as discussed in [3] hence supports this line of research.

To the best of our knowledge, there have been no attempts to exploit the acyclicity property as is done in this paper.

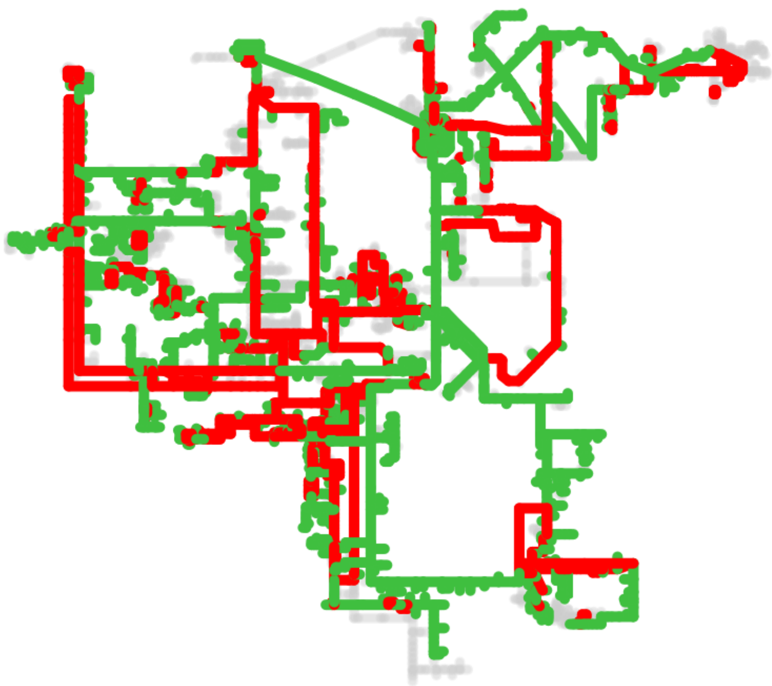


Figure 1: Tightness of the flow bounds obtained for a large-scale meshed gas network.

The remaining paper is structured as follows. Section 1 discusses two common relaxations used to solve potential-driven network flow problems in practice and why the presence of cycles in the network weakens these relaxations. In Section 2, we derive our combinatorial relaxation from a generic MINLP containing the potential-driven network flow problem as a submodel. Section 3 shows how this combinatorial relaxation can be used to strengthen the original model. We present some preliminary computational results indicating the impact of this approach in Section 4 and provide some conlusions Section 5.

1 Weak relaxations on meshed networks

In this section we study the quality of two common relaxations on the large-scale real-world network shown in Figure 1. It is well-known [24] that meshed gas networks are much harder to optimize than tree networks or networks with very few cycles. The common sense explanation is that on trees, all flows are fixed while networks with cycles admit different flow vectors (in principle; for networks without active elements the flow vector may be unique inspite of cycles [21, 5]). Our analysis provides another complementing explanation for the difficulty incurred by cycles: The relaxations used for global optimization do not incoporate the acyclicity property which is only relevant on meshed (and sufficiently large) networks.

1.1 Relaxation 1: Classical network flow problem

The relaxation consists of just the flow conservation constraints (1b) and the flow bounds (1d). It is useful e.g., for bound tightening [25], where the flow over each arc is maximized and minimized to obtain improved flow bounds for this arc.

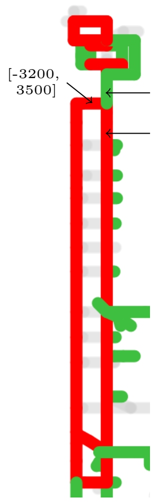
Figure 2a shows a subnetwork of a real-world gas network that contains a cycle. In this case, the cycle arises due to two pipelines running in parallel, which is very common for high-load transmission systems. Note that there are several short pipe segments along the right pipeline which are used to route some of the transmissioned gas to customers. Depending on the demand situation, the parallel pipes may not be operated in parallel, i.e., the gas is flowing in different directions. However, for the demand vector considered here, the pipes can be operated in parallel.

We performed the bound tightening for the flow bounds as explained above. The colors in the picture indicate whether this bound tightening was able to fix the flow direction (green arcs) or not (red arcs). Obviously, the flow directions could not be infered for the red cycles. The reason is that when e.g., maximizing the flow along a given arc, in the classical network flow problem it is possible and beneficial to send as much flow as possible along the cycle to get a large flow on each arc. When minimizing the flow, basically the same amount is send in the opposite direction. However, this is an unphysical solution that is not feasible for the potential-driven network flow problem. Thus the flow bounds of $[-3200, 3500]$ obtained for each arc of the big cycle are very weak. In fact, the 309 flow units arriving from the top have to be routed to the bottom, so this is an upper bound for the flow along each of the two pipes. To obtain this result from the bound tightening problem, one has to include some constraint to forbid flow along cycles.

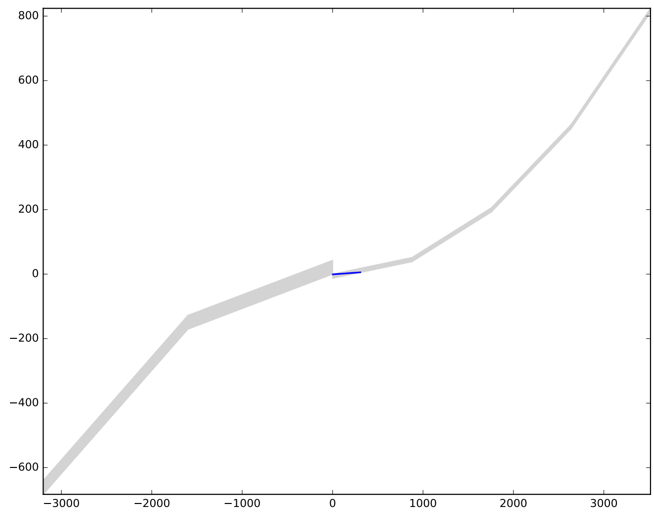
1.2 Relaxation 2: (piecewise) Linear relaxation

In this relaxation, the nonlinear constraints are replaced by (piecewise) linear functions such that the resulting feasible region contains the original one. The corresponding MILP model can be constructed once and then solved with a standard solver [8, 7]. Alternatively, state-of-the-art MINLP solvers like SCIP [1] or BARON [2] construct such a linear relaxation in each search tree node dynamically according to the current variable bounds.

Figure 2b shows the piecewise linear relaxation (grey area) constructed with the techniques from [8] for the potential loss function of one of the arcs on the big cycle. To construct this relaxation, the weak bounds from the classical network flow problem have been used. The small blue area indicates the piecewise linear relaxation that can be constructed from the tighter bounds of $[0, 309]$. In this case, one piecewise linear segment instead of six is sufficient. Moreover, the area of the relaxation is significantly reduced, indicating a much stronger relaxation. Again, to obtain this strong relaxation it is necessary to disallow flow along cycles.



(a) Subnetwork with cycles.



(b) Piecewise linear relaxation for potential loss on arc with loose flow bounds.

Figure 2: Example for which the network flow relaxation yields weak bounds.

2 Acyclic flow orientations as combinatorial relaxations for potential-driven network flow problems

The aim of this section is to derive a combinatorial relaxation capturing the acyclicity property implied by potential-driven flows and the flow balance property at the same time. Potential-driven network flow problems usually occur as submodels in networks with additional elements. In order to exploit this structure on a subnetwork that is as large as possible, we consider models for further network elements for which the acyclicity property also holds.

In particular, we consider a network represented as a directed graph $(V, A_{\text{pi}} \cup A_{\text{sp}} \cup A_{\text{va}} \cup A_{\text{cv}} \cup A_{\text{other}})$, where the arc set is partitioned in the following arc subsets:

pipes A_{pi} network elements with potential loss described by the potential loss function $\phi_a(q_a)$, where q_a denotes the flow along $a \in A_{\text{pi}}$

short pipes A_{sp} network elements without any potential loss (which are often used for modeling purposes and thus considered here),

valves A_{va} network elements that can be open or closed, either admitting flow without potential loss or blocking flow, respectively,

control valves A_{cv} network elements that allow to reduce the potential in a controllable way,

other network elements A_{other} network elements of other types, e.g., compressors or pumps.

Although our terminology for the network elements is clearly inspired by gas networks, the MINLP model considered below is rather generic. Our results can thus readily be applied to other problems from this class, e.g., to water networks.

The operation of each network element $a = uv \in A$ is described by the feasible set $F_a \subseteq \{(\pi_u, \pi_v, q_a) \in \mathbb{R}^3 \mid \pi_u, \pi_u \geq 0\}$ relating the feasible values of the inlet potential π_u, the outlet potential π_v, and the flow q_a. For technical reasons, we are only able to handle elements with certain properties. First of all, we require the potential loss function ϕ_a of each pipe $a \in A_{\mathrm{pi}}$ to have the following properties:

$$\phi_a(q_a) \geq 0 \implies q_a \geq 0, \tag{2a}$$
$$\phi_a(q_a) \leq 0 \implies q_a \leq 0, \tag{2b}$$
$$\phi_a(q_a) = 0 \implies q_a = 0. \tag{2c}$$

Moreover, we consider the following two types of special control valves, both of which admit only nonnegative flow.

control valves of type I always strictly reduce the potential. Formally, the feasible set F_a has the following property:

$$F_a \subseteq \{(\pi_u, \pi_v, q_a) \in \mathbb{R}^3_{\geq 0} \mid \pi_u > \pi_v\}. \tag{3}$$

control valves of type II allow to maintain the potential for "small" flows. Formally, the feasible set F_a has the following properties:

$$F_a \subseteq \{(\pi_u, \pi_v, q_a) \in \mathbb{R}^3_{\geq 0}\}, \tag{4a}$$
$$(\pi_u, \pi_u, q_a) \in F_a \text{ and } 0 \leq q'_a \leq q_a \implies (\pi_u, \pi_u, q'_a) \in F_a. \tag{4b}$$

In the following, we assume that the set A_{cv} consists only of control valves of these two types. Control valves of differing types and further network elements can be included in the set A_{other} to treat them within our framework.

Remark 1 Observe that the only switched elements here are the valves and the remaining controllable elements (control valves, compressors) are always "active". Additional states ("closed", "bypass") as considered e.g., in [20] can be modeled using additional valves and short pipes and are thus also captured by the model. □

We consider the following generic MINLP for potential flow problems.

$$\min \quad c^T(q, \pi, s) \tag{5a}$$
$$q_v^{\mathrm{nom}} + \sum_{a=uv \in A} q_a - \sum_{a=vu \in A} q_a = 0 \quad \text{for all } v \in V, \tag{5b}$$
$$\pi_u - \pi_v = \phi_a(q_a) \quad \text{for all } a \in A_{\mathrm{pi}}, \tag{5c}$$
$$\pi_u - \pi_v = 0 \quad \text{for all } a \in A_{\mathrm{sp}}, \tag{5d}$$
$$s_a = 0 \implies q_a = 0, \quad \text{for all } a \in A_{\mathrm{va}}, \tag{5e}$$
$$s_a = 1 \implies \pi_u = \pi_v, \quad \text{for all } a \in A_{\mathrm{va}}, \tag{5f}$$
$$(\pi_u, \pi_v, q_a) \in F_a \quad \text{for all } a \in A_{\mathrm{cv}}, \tag{5g}$$
$$(\pi_u, \pi_v, q_a) \in F_a \quad \text{for all } a \in A_{\mathrm{other}}, \tag{5h}$$
$$\underline{q}_a \leq q_a \leq \overline{q}_a \quad \text{for all } a \in A, \tag{5i}$$
$$\underline{\pi}_u \leq \pi_u \leq \overline{\pi}_u \quad \text{for all } u \in V. \tag{5j}$$

Observe that although (5g) and (5h) are formally the same, we actually require the feasible sets F_a of control valves to satisfy one of the conditions (3) or (4) according to their type. In contrast, the set F_a of network elements in A_{other} may be arbitrary. In particular, increasing the potential is allowed. This may lead to cyclic flows, which is the main reason why these elements are treated specially (i.e., ignored in the relaxation to be constructed).

Our first result establishes that under suitable assumptions on the cost vector, the MINLP (5) always has an optimal solution that is an acylic flow as defined next.

Definition 1 Let $q\colon A \to \mathbb{R}$ be a flow on a digraph $D = (V, A)$ for a supply vector q^{nom}, i.e., q satisfies (5b). The flow q is called an *acyclic flow* if there is a bijective mapping $\sigma\colon V \to \{1, \ldots, |V|\}$ satisfying

$$\begin{aligned} \sigma(u) > \sigma(v) &\implies q_a \geq 0 \\ \sigma(u) < \sigma(v) &\implies q_a \leq 0 \end{aligned} \quad \text{for all } a = uv \in A. \tag{6}$$

A mapping σ satisfying (6) is called an *acyclic node ordering* for the flow q. □

An acyclic node ordering σ for a given flow induces an orientation $D^\sigma = (V, A^\sigma)$ of the original digraph $D = (V, A)$ via

$$A^\sigma := \{uv \mid uv \in A,\, \sigma(u) > \sigma(v)\} \cup \{vu \mid uv \in A,\, \sigma(v) > \sigma(u)\}. \tag{7}$$

Observe that D^σ is an acyclic digraph as (7) states that σ is a topological sorting for D^σ. The oriented flow $q^\sigma\colon A^\sigma \to \mathbb{R}$ defined by

$$q^\sigma_a := \begin{cases} q_a & a = uv, \\ -q_a & a = vu \end{cases} \quad \text{for all } a \in A$$

is then a non-negative flow in the acyclic digraph D^σ – hence the name *acyclic flow.*

Theorem 1 *Consider a MINLP* (5) *for a digraph* $D = (V, A)$ *and a supply vector* q^{nom}*. Let* $\tilde{D} = (V, \tilde{A})$ *be the subgraph of* D *defined by*

$$\tilde{A} := A \setminus \Big(A_{\text{other}} \cup \{a \in A_{\text{sp}} \cup A_{\text{va}} \cup A_{\text{cvII}} \mid c_{q_a} \neq 0\}\Big), \tag{8}$$

where A_{cvII} *denotes the set of control valves of type II. Then there is an optimal solution* (q^*, π^*, s^*) *of* (5) *such that* q^* *is an acyclic flow on* $\tilde{D}$*.* □

Proof Let (q, π, s) be a feasible solution of (5) for D. Without loss of generality, we can assume that all arcs are oriented such that $q_a \geq 0$ (by changing the direction of the arc and the sign of the flow, which does not affect the truth of (6)).

To define a suitable node order σ, let $\mathcal{L} := \{\pi_u \mid u \in V\}$ be the set of potential levels in the solution. We partition the node set by the potential levels by defining node sets $V_\ell := \{u \in V \mid \pi_u = \ell\}$ for all $\ell \in \mathcal{L}$. This node partition induces a partition of the arcs $\tilde{A}$ into *potential-reducing arcs* and *potential-maintaining arcs.*

The ordering σ is defined such that

$$\sigma(u) > \sigma(v) \text{ whenever } \pi_u > \pi_v, \tag{9}$$

which prescribes the orientation of the potential-reducing arcs. Consider a potential-reducing arc $a = uv$. For a pipe $a \in A_{\text{pi}}$, the relation $\pi_u > \pi_v$ implies $q_a \geq 0$, due to the required properties (2) of the potential loss function. Moreover, the arc a cannot be a short pipe nor an open valve due to (5d) and (5f), respectively. For a closed valve $a \in A_{\text{va}}$, we have $q_a = 0$. If $a \in A_{\text{cv}}$ we must have $\pi_u > \pi_v$ and $q_a \geq 0$ by (3) and (4). We thus established (6) for the potential-reducing arcs.

It remains to define the order of the nodes within each V_ℓ. If there is an ordering that satisfies (9) and, additionally,

$$\sigma(u) > \sigma(v) \iff q_a > 0 \quad \text{for all } a = uv \in \tilde{A} \text{ with } u, v \in V_\ell \text{ and } q_a > 0 \quad (10)$$

for any $\ell \in \mathcal{L}$, (6) obviously holds. Assume that (q, π) does not fulfill (10). Then there exists a cycle, i.e., a sequence of arcs $a_1 = (u_1, u_2), a_1 = (u_2, u_3), \ldots, a_k = (u_k, u_1)$, with $q_{a_i} > 0$ for every $1 \leq i \leq k$. Due to the properties (2) of the potential loss function, $q_{a_i} > 0$ implies $a_i \notin A_{\text{pi}}$. Likewise, a_i cannot be a closed valve or a control valve of type I. Hence, a_i is either a short pipe, an open valve, or a control valve of type II. We can thus reduce the flow along the cycle until the flow along one arc becomes 0 without affecting the feasiblity or the cost (hence the exclusion of arcs of these types with nonzero cost from $\tilde{A}$). Repeated application of this operation breaks the cycle and yields a flow q' for which (10) is fulfilled. Since the flow adjustment affects only potential-maintaining arcs, the above argument for the potential-reducing arcs holds for q' as well. Moreover, (10) implies (6) for the corresponding arcs.

Finally, (6) can obviously be satisfied for any of the remaining arcs $a = uv$ with $q_a = 0$ by chosing any ordering of u and v that is consistent with (9) and (10). ■

Theorem 1 implies that the MINLP (5) complemented by the constraint

$$\{q \colon A \to \mathbb{R} \mid q \text{ is acyclic on } \tilde{D}\} \quad (11)$$

is equivalent to (5) in the sense that one of the two problems is feasible iff the other one is feasible and both problems have the same objective value. Thus any relaxation of (5) can be strengthened (in this sense of solution equivalence) by adding (a relaxation of) constraint (11). However, it is nonobvious how to express (11) (or a relaxation) in a mathematical program. In the following, we develop a purely combinatorial relaxation of (11) and flow conservation (5b) that can be formulated using additional binary variables and additional constraints. For this relaxation, we assume that for each network element a, finite lower and upper bounds $\underline{q}_a$ and $\overline{q}_a$ for the flow are known. These can be obtained e.g., via standard bound-tightening techniques as described e.g., in [25]. Moreover, we also treat q^{nom} as a variable with lower and upper bounds $\underline{q}^{\text{nom}}$ and $\overline{q}^{\text{nom}}$.

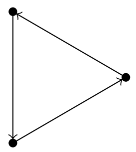
From now on, we assume that the arcs of the digraph $D = (V, A)$ are oriented in the direction of the flow if the direction is already known.

Assumption 1 *Let $\underline{q}$ and $\overline{q}$ be valid bounds for the flows along each arc for any supply vector with $\underline{q}^{\text{nom}} \leq q^{\text{nom}} \leq \overline{q}^{\text{nom}}$. For each network element a, these flow bounds either satisfy $\underline{q}_a < 0 < \overline{q}_a$ or $0 \leq \underline{q}_a$.*

In case this assumption is not fulfilled (i.e., there is an arc with $\overline{q}_a < 0$), it can be met by reversing this arc and adjusting the flow bounds accordingly.

The basic idea of this combinatorial relaxation is to model the arc orientations that may occur in solutions of (5) as orientations of a graph. Theorem 1 implies that it is sufficient to consider orientations that are acyclic. To take into account flow conservation as well, it is tempting to require that in addition to being acyclic, each node has to have at least one in-arc and one out-arc (adjusting for sources and sinks, which would count as in-arc and out-arc, respectively). However, these requirements together may be inconsistent, as shown by the following counterexamples, for both of which the zero flow is a feasible (acyclic) solution.

Example 1 (3-cycle with no sources and sinks) All of the nodes have to have an in-arc and an out-arc, but this yields a cycle:



□

Example 2 (K_4 with no sources and sinks) Having an orientation that satisfies the above requirements, reverting the orientations of all arcs yields an orientation that satisfies them, too. Therefore, we can wlog assume that the node 1 has an in-arc and two out-arcs. By symmetry, we can assume that the out-arcs are nodes 2 and 3. Then the edge $\{2,4\}$ needs to be oriented as $(4,2)$, since otherwise there is a cycle. Now there are the two in-arcs $(1,2)$ and $(4,2)$ at node 2, thus the edge $\{2,3\}$ must be the out-arc $(2,3)$. Orienting the remaing edge either yields a cycle or violates the combinatorial supply/demand constraints. □

Thus more refined criteria are necessary to handle zero flows. To describe these, some more notation is necessary. We use the arc flow bounds to restrict the possible directions of each arc. The bounds for the supply at a node indicate whether the node may be a source or a sink. It will later be useful to consider subdigraphs defined by subsets of the arcs. For these subdigraphs, we use adjusted bounds for the supply at the nodes. The intuition is that flow leaving (entering) a node on arcs that are not part of the considered subdigraphs lets the node work as a sink (source) for the subdigraph.

Definition 2 Let $\underline{q}$ and $\overline{q}$ be lower and upper bounds for the flow on each arc and $\underline{q}^{\text{nom}}$ and $\overline{q}^{\text{nom}}$ be lower and upper bounds on the supply at each node. The *set of valid directions* $\Delta(a)$ of an arc $a \in A$ is the minimum set satisfying

$$\overline{q}_a > 0 \implies \mathsf{fwd} \in \Delta(a), \tag{12a}$$

$$\underline{q}_a < 0 \implies \mathsf{bwd} \in \Delta(a), \tag{12b}$$

$$0 \in [\underline{q}_a, \overline{q}_a] \implies \mathsf{0} \in \Delta(a). \tag{12c}$$

For a subset $A' \subseteq A$, the *supply bounds induced by* A' for a node $v \in V$ are given by

$$\underline{q}_v^{\text{nom},A'} := \underline{q}_v^{\text{nom}} + \sum_{a=uv \in A \setminus A'} \underline{q}_a - \sum_{a=vu \in A \setminus A'} \overline{q}_a, \tag{13a}$$

$$\overline{q}_v^{\text{nom},A'} := \overline{q}_v^{\text{nom}} + \sum_{a=uv \in A \setminus A'} \overline{q}_a - \sum_{a=vu \in A \setminus A'} \underline{q}_a. \tag{13b}$$

$\square$

The following definition and result provide the desired combinatorial relaxation of acyclic flows.

Definition 3 Consider a MINLP (5) for a digraph $D = (V, A)$ and assume that $\underline{q}$ and $\overline{q}$ are valid bounds for the flows along each arc for any supply vector with $\underline{q}^{\text{nom}} \leq q^{\text{nom}} \leq \overline{q}^{\text{nom}}$. Let $A' \subseteq A$ be a subset of the arcs. A digraph $\vec{D} = (V, A'_{\omega,\rightleftarrows} \cup A'_{\omega,\mathsf{0}})$ defined by a mapping $\omega\colon A' \to \{\mathsf{fwd}, \mathsf{bwd}, \mathsf{0}\}$ via

$$
\begin{aligned}
A'_{\omega,\mathsf{fwd}} &:= \{uv \mid a = uv \in A', \omega(a) = \mathsf{fwd}\}, && \text{(14a)}\\
A'_{\omega,\mathsf{bwd}} &:= \{vu \mid a = uv \in A', \omega(a) = \mathsf{bwd}\}, && \text{(14b)}\\
A'_{\omega,\mathsf{0}} &:= \{uv \mid a = uv \in A', \omega(a) = \mathsf{0}\}, && \text{(14c)}\\
A'_{\omega,\rightleftarrows} &:= A'_{\omega,\mathsf{fwd}} \cup A'_{\omega,\mathsf{bwd}}, && \text{(14d)}
\end{aligned}
$$

is called an *acyclic flow orientation for A'*, if

(AFO-1) The direction of each arc $a \in A'$ is a valid direction conforming to the flow bounds, i.e., $\omega(a) \in \Delta(a)$.

(AFO-2) The subdigraph $\big(V, A'_{\omega,\rightleftarrows} \cap \tilde{A}\big)$ is acyclic.

(AFO-3) Each node $v \in V$ incident to $A'_{\omega,\rightleftarrows}$ has at least one in-arc and one out-arc (with possibly positive supply counting as in-arc, and possibly negative supply counting as out-arc):

$$
\begin{aligned}
|\{uv \in A'_{\omega,\rightleftarrows}\}| + \mathbb{1}_{\overline{q}_v^{\text{nom},A'} > 0} &\geq 1, && \text{(15a)}\\
|\{vu \in A'_{\omega,\rightleftarrows}\}| + \mathbb{1}_{\underline{q}_v^{\text{nom},A'} < 0} &\geq 1. && \text{(15b)}
\end{aligned}
$$

Arcs in $A'_{\omega,\mathsf{fwd}}$, $A'_{\omega,\mathsf{bwd}}$, and $A'_{\omega,\mathsf{0}}$ are called *forward arcs*, *backward arcs*, and *zero arcs*, respectively. $\square$

Theorem 2 *Let (q, π, s) be a solution of the MINLP* (5) *augmented with constraint* (11)*. For every arc subset $A' \subseteq A$, the digraph $\vec{D} = (V, A'_{\omega,\rightleftarrows} \cup A'_{\omega,\mathsf{0}})$ defined by*

$$
\omega_q(a) := \begin{cases} \mathsf{fwd} & q_a > 0, \\ \mathsf{bwd} & q_a < 0, \\ \mathsf{0} & q_a = 0, \end{cases} \qquad \textit{for all } a = uv \in A'. \tag{16}
$$

is an acyclic flow orientation for A'. $\square$

Proof For $A' = A$, the mapping ω_q satisfies requirement (AFO-1), as q is a feasible and thus respects the flow bounds on each arc. Likewise, requirement (AFO-2) is satisfied due to constraint (11). Therefore, both requirements are also satisfied for every proper subset of A.

It remains to establish requirement (AFO-3) for an arbitrary $A' = A$. Consider an arc $a \in A'_{\omega,\rightleftarrows}$ incident to node v. Assume that $a \in A'_{\omega,\mathsf{fwd}}$, i.e., $q_a > 0$, and $a = uv$. In this case, (15a) is obviously fulfilled, as the first term is at least 1. Moreover, condition (15b) is satisfied, too, if there is another arc $a' = vw \in A'_{\omega,\rightleftarrows}$. Assume that this is not the case, i.e., $|\{vw \in A'_{\omega,\rightleftarrows}\}| = 0$. Due to the definition of ω_q this implies

$$\sum_{a'=vw\in A'} q_{a'} \le 0, \quad \text{and} \quad \sum_{a'=wv\in A',\, a'\neq a} q_{a'} \ge 0,$$

i.e., all arcs in A' that are incident to v carry flow into node v. Thus this flow and the positive flow from arc a has to leave node u as negative supply (either because u is a sink or on arcs not contained in A'). Formally, the lower supply bound induced by A' is negative:

$$\begin{aligned}
\underline{q}_v^{\text{nom},A'} &= \underline{q}_v^{\text{nom}} + \sum_{a'=wv\in A\setminus A'} \underline{q}_{a'} - \sum_{a'=vw\in A\setminus A'} \overline{q}_{a'} \\
&\le q_v^{\text{nom}} + \sum_{a'=wv\in A\setminus A'} q_{a'} - \sum_{a'=vw\in A\setminus A'} q_{a'} \\
&= -q_a - \sum_{a'=wv\in A',\, a'\neq a} q_{a'} + \sum_{a'=vw\in A'} q_{a'} \\
&\le -q_a < 0.
\end{aligned}$$

This establishes condition (15b) in the case $|\{vw \in A'_{\omega,\rightleftarrows}\}| = 0$.

The case $a \in A'_{\omega,\mathsf{fwd}}$ and $a = vw$ works the other way around: Condition (15b) is obviously fulfilled and condition (15a) is derived from that. The same arguments apply in the cases for $a \in A'_{\omega,\mathsf{bwd}}$. ■

Theorem 2 implies that a strengthening of constraint (11) is given by

$$\{q\colon A' \to \mathbb{R} \mid \omega_q \text{ as defined by (16) yields an acyclic flow orientation}\} \tag{17}$$

for $A' = A$. By choosing any arc subset $A' \subseteq A$, a relaxation of (17) may be obtained.

We will now discuss how to incorporate Constraint (17) in optimization models.

3 Exploiting acyclic flow orientations to improve relaxations

As discussed in the introduction, the fact that the potential-driven network flow submodel does not admit cyclic flows is not necessarily reflected in the relaxations used. To incorporate this fact in relaxation models, one may add Constraint (17). In the following, we describe models for (17) that are supposed to be used as submodels *in addition* to relaxation model considered. We assume that the relaxation model contains at least the flow variables, which are further constrained.

We will begin by addressing the question of how to model the orientation of a single arc. In Examples 1 and 2 in the previous section we have seen that there are graphs that do not allow for an orientation that is acyclic and where each node has both at least one in-arc and one out-arc (adjusting for sources and sinks, which would count as in-arc and out-arc, respectively). For this reason our concept of an *acyclic flow orientation* introduced three types of arcs: forward arcs, backward arcs and zero arcs.

Within the framework of a MINLP this raises the question of how to model these three possible orientations of an arc. Using a model with three different orientations for each arc may lead to a unnecessarily large number of possible orientations of a graph, which is likely to be computationally very expensive. Moreover, two binary variables are needed for each arc.

Fortunately, we can draw on two results from [3] to simplify the situation.

Theorem 3 *The arc subset $\tilde{A}$ of any directed graph $D = (V, A)$ can be decomposed into two disjoint (possibly empty) sets $\tilde{A}_0 \cup \tilde{A}_{\rightleftarrows} = \tilde{A}$ such that for each feasible solution of the MINLP* (5) *we have*

1. $q_a = 0$ *for all* $a \in \tilde{A}_0$, *and*
2. *there exists an acyclic flow orientation ω for $\tilde{A}$ with $\tilde{A}_{\omega,\rightleftarrows} = \tilde{A}_{\rightleftarrows}$ (i.e., all arcs in $\tilde{A}_{\rightleftarrows}$ are either forward or backward arcs) and*

$$\omega(a) = \mathsf{fwd} \implies q_a \geq 0,$$
$$\omega(a) = \mathsf{bwd} \implies q_a \leq 0. \qquad \square$$

Proof Follows from Corollaries 5 and 6 in [3]. ■

The previous Theorem 3 implies that for each network there exist acyclic flow orientations without zero arcs for a subset $\tilde{A}_{\rightleftarrows}$ of the arcs, while we can determine in advance that all flows on the arcs $\tilde{A}_0$ must be zero. (For instance, in the examples above we have $A = \tilde{A}_0$.) Moreover, the forward and backward direction of an arc in an acyclic flow orientation corresponds to the sign of the flow variable of at least one feasible solution. Hence we can model the constraint (17) imposed by the acyclic flow orientations as follows.

The arcs in the set $\tilde{A}_0$ are handled by the trivial constraint

$$q_a = 0 \quad \text{for all } a \in \tilde{A}_0. \tag{18}$$

The choice of the forward or backward direction for the arcs in $\tilde{A}_{\rightleftarrows}$ can be formulated by introducing binary variables x_a for the flow direction of each arc $a = uv \in \tilde{A}_{\rightleftarrows}$, where $x_a = 1$ means flow from u to v and $x_a = 0$ indicates flow in the opposite direction. The coupling between these binary variables and the corresponding flow variables can be achieved via the big-M constraints

$$\underline{q}_a(1 - x_a) \leq q_a \leq \overline{q}_a x_a \quad \text{for all } a \in \tilde{A}_{\rightleftarrows}. \tag{19}$$

One option to model the requirements for an acyclic flow orientation on the arcs $\tilde{A}_{\rightleftarrows}$ is to use a suitable MILP model for the degree requirement (AFO-1) and to model the acyclicity requirement (AFO-2) via the constraints for the acyclic subgraph polytope [15]. However, we expect this approach not to be computationally effective.

Instead, we employ a Dantzig-Wolfe reformulation: We enumerate all possible acyclic flow orientations and require that one of those acyclic flow orientations is chosen. Of course, this approach will not work for large networks as we expect the number of acyclic flow orientations to grow exponentially in the number of arcs. For this reason, we consider a family $\mathcal{C} = \{C_1, \dots, C_k\}$ of subsets of $\tilde{A}$ for which all acyclic flow orientations can be enumerated with reasonable effort. Observe that in general, this does not guarantee that an acyclic flow orientation for the entire set $\tilde{A}$ is chosen.

Let $\mathcal{O}_i$, $1 \le i \le k$, be the set of orientations for the arc subset C_i. For each $\tilde{D} \in \mathcal{O}_i$ we introduce a binary variable $y^C_{\tilde{D}}$, where $\tilde{D}$ is selected iff $y^C_{\tilde{D}} = 1$. This requirement is formulated as

$$\sum_{\tilde{D} \in \mathcal{O}\colon a \text{ is forward arc}} y^C_{\tilde{D}} = x_a \quad \text{for all } a \in \tilde{A} \cap C, C \in \mathcal{C}. \tag{20}$$

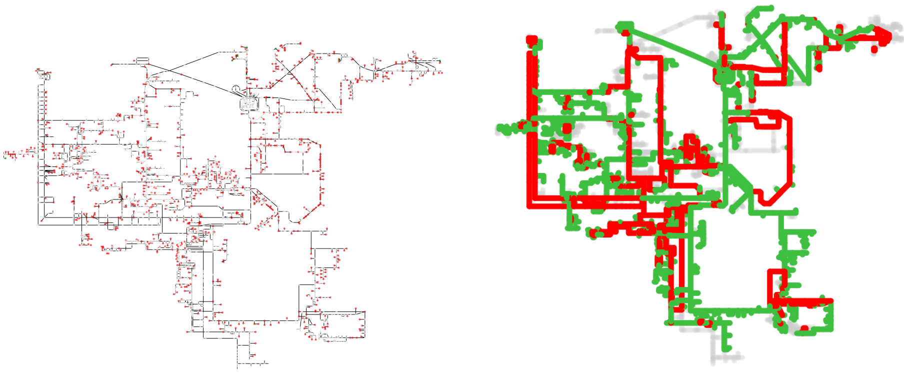
Constraints (18), (19), (20) provide a MILP formulation of Constraint (17). Note that this formulations involves many additional binary variables which may substantially increase the solving time for the relaxation. To benefit to some extent from the knowledge about the acyclic flow orientations it is also possible to relax the integrality requirement for the variables $y^C_{\tilde{D}}$, yielding a weaker relaxation.

4 Preliminary computational results

In order to investigate the computational potential of these ideas we consider a single supply vector q^{nom} for the real-world network shown in Figure 3a. Our aim is to improve the two relaxations discussed in Section 1. Hence we perform the bound tightening implemented during the FORNE project [20] as summarized in [25]. Among other bound tightening techniques, this includes optimality-based bound tightening for the flows, i.e., minimizing and maximizing the flow over each arc subject to flow conservation constraints and flow bounds (either from the original input or derived via other bound tightening steps). This bound tightening is able to fix the flow direction on a large share of the network arcs (colored green in Figure 3b), but there also remain large parts of the network where the flow direction cannot be fixed (colored red in Figure 3b). Incidentally, these tend to be the main trannsmission lines since these are often part of a cycle.

We choose the subsets of $\tilde{A}$ for which we enumerate acyclic flow orientations to be the components of the graph consisting of the arcs for which the flow direction could not be fixed. For each arc subset $A' \subseteq \tilde{A}$, we construct the undirected graph induced by this arc subset, designating nodes as sources or sinks according to the induced supply bounds computed via to (13). We apply the enumeration algorithm from [3] to obtain the set of acyclic flow orientations for this undirected graph. These sets of acyclic flow orientations are then used to set up a bound-tightening MILP consisting of the original flow conservation constraints, flow bounds derived via the original bound tightening procedure, and Constraints (18), (19), (20). This MILP is solved twice for each arc, minimizing and maximizing the flow over the arc, respectively.

Table 1 presents the improvement of the flow bounds obtained by this method. The first line shows that the number of arc where the flow could be fixed to zero increases by 55. The following lines show the number of arcs for which the *flow range*, the difference between the upper and the lower flow bound for this arc, exceeds a certain threshold. (To relate the size of the threshold, note that the total supply transmissioned through the network is roughly 3500



(a) A real-world large-scale gas network.

(b) Components (red) where the existing bound tightening does not fix the flow direction.

Figure 3: A real-world large-scale gas network and results of bound tightening for the considered supply vector.

units.) It is evident that the number of arcs which huge flow range can be reduced significantly. These results show that the proposed technique is able to significantly strengthen the classical network flow relaxation.

Table 2 presents the impact of the tighter flow bounds on the size of a piecewise linear relaxation constructed with the method from [7, 8]. The size is measured as the number of binary variables used to model the choice between piecewise linear segments (which is equal to the number of this segments). To measure the quality of the relaxation, we compute the total area of the piecewise linear segments. Note these are relaxations of nonlinear function and thus the "true" area of the feasible region is 0.0. Shown is the impact for the two main classes of nonlinear functions from the models considered. The function $q_a|q_a|$ is the potential loss function for gas networks, whereas the function $p_u \leftrightarrow \pi_u$ maps the pressure of the node to its potential (being the square of the pressure). Clearly, the improved bounds yield also significantly tighter piecewise linear relaxations.

5 Conclusions and further work

We proposed acyclic flow orientations as a combinatorial relaxation capturing essential properties of feasible solutions of potential-driven flow problems. Incorporating the restriction to acyclic flow orientations into established relaxations leads to tighter relaxations, promising a significant computational advantage.

To fully benefit from this, it is necessary to understand the structure of acyclic flow orientations and how to enumerate them. This theory is provided by the companion report [3]. The next step will be an extensive computational evaluation of the impact of exploiting acyclic flow orientations to solve MINLPs with a potential-driven network flow submodel. It is to be expected that the enumeration of acyclic flow orientations for bigger subgraphs is prohibitive, so the choice of suitable subgraphs is likely to be crucial. Our initial results for considering the subgraphs of arcs with open flow direction show that a substantial

flow range	original	# arcs with orientations	rel. reduction
= 0.0	1057	1112	5.20%
≥ 1000	430	294	-31.63%
≥ 2000	373	263	-29.49%
≥ 3000	286	211	-26.22%
≥ 4000	173	40	-76.88%
≥ 5000	154	14	-90.91%
≥ 6000	146	9	-93.84%
≥ 7000	47	9	-80.85%

Table 1: Results of bound tightening strengthened by acyclic flow orientations. "flow range" is the difference between the upper and the lower bound derived for the flow along an arc. The flow direction could be fixed for 143 out of the 1260 arcs for which the flow direction could not be determined before.

	original		with orientations		improvement	
	#bin vars	∅ area	#bin vars	∅ area	#bin vars	∅ area
function type						
$q_a\|q_a\|$	4450	9195.85	3602	3171.98	-19.06%	-65.51%
$p_u \leftrightarrow \pi_u$	1586	331.32	1412	307.26	-10.97%	-7.26%

Table 2: Impact of the improved flow bounds on the size and quality of a piecewise linear relaxation.

improvement can already be gained by considering small subgraphs.

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