Gas Transport Network Optimization: Mixed-Integer Nonlinear Models

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1. Introduction

Although modern societies strive towards energy systems that are entirely based on renewable energy carriers, natural gas is still one of the most important energy sources. This became even more obvious in Europe with Russia's 2022 war against the Ukraine and the resulting stop of gas supplies from Russia. Besides that it is very important to use this scarce resource efficiently. To this end, it is also of significant relevance that its transport is organized in the most efficient, i.e., cost- or energy-efficient, way. The corresponding mathematical optimization models have gained a lot of attention in the last decades in different optimization communities. These models are highly nonlinear mixed-integer problems that are constrained by algebraic constraints and partial differential equations (PDEs), which usually leads to models that are not tractable. Hence, simplifications have to be made and in this chapter, we present a commonly accepted finite-dimensional stationary model, i.e., a model in which the steady-state solutions of the PDEs are approximated with algebraic constraints. For more details about the involved PDEs and the treatment of transient descriptions we refer to Hante and Schmidt [16]. The presented finite-dimensional as well as mixed-integer nonlinear and nonconvex model is still highly challenging if it needs to be solved for real-world gas transport networks. Hence, we also review some classic solution approaches from the literature.

The research on optimizing gas transport networks started in the late 1960s with the works [34, 35] and is still going on; see, e.g., the book [18], the survey [28], or the overview book chapter [13].

2. Modeling

Gas transport networks are typically modeled as directed and weakly connected graphs $G = (\mathcal{V}, \mathcal{A})$ with node set $\mathcal{V}$ and arc set $\mathcal{A}$. For stationary descriptions, the nodes are split in so-called entries $\mathcal{V}_+$ at which gas is supplied, exits $\mathcal{V}_-$ at which gas is withdrawn, and inner nodes $\mathcal{V}_0$ at which neither gas is supplied nor withdrawn. Thus, we have $\mathcal{V} = \mathcal{V}_+ \cup \mathcal{V}_- \cup \mathcal{V}_0$. The arcs are used to model the different elements of gas transport networks. In this chapter, we focus on pipes $\mathcal{A}_{\mathrm{pi}}$, compressors $\mathcal{A}_{\mathrm{co}}$, control valves $\mathcal{A}_{\mathrm{cv}}$, and valves $\mathcal{A}_{\mathrm{vl}}$. In reality, there are also filters, chromatographs, etc. but we present a model in what follows for the setting in which $\mathcal{A} = \mathcal{A}_{\mathrm{pi}} \cup \mathcal{A}_{\mathrm{co}} \cup \mathcal{A}_{\mathrm{cv}} \cup \mathcal{A}_{\mathrm{vl}}$ holds. This represents what is commonly done in the mathematical optimization literature.

Next, we briefly discuss some basic models for the different elements in the network. To this end, we need some fundamental quantities to describe gas physics. When we discuss stationary models, i.e., neglect all dynamic effects, the main variables are the gas mass flow q_a on arcs $a \in \mathcal{A}$ and the gas pressure p_u on all

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nodes $u \in \mathcal{V}$. Since we restrict ourselves to the case of isothermal models, the gas temperature T is considered to be a network-wide constant. With these assumptions, the gas velocity and the gas density get dependent variables that can be computed from these quantities. Details and instationary models are discussed in [16].

2.1. **Nodes.** Nodes are modeled as elements without spatial dimension that cannot store gas. Hence, they are mainly modeled using a mass balance constraint

$$\sum_{a \in \delta^{\text{out}}(u)} q_a - \sum_{a \in \delta^{\text{in}}(u)} q_a = q_u, \quad u \in \mathcal{V}.$$

Here, $\delta^{\text{in}}(u)$ and $\delta^{\text{out}}(u)$ are the sets of all in- and outgoing arcs of node u and q_u is the amount of supplied or withdrawn gas at node u, i.e., it holds

$$q_u \begin{cases} \geq 0, & \text{if } u \in \mathcal{V}_+, \\ \leq 0, & \text{if } u \in \mathcal{V}_-, \\ = 0, & \text{if } u \in \mathcal{V}_0. \end{cases}$$

Finally, the gas pressure variables p_u are bounded:

$$0 < p_u^- \leq p_u \leq p_u^+, \quad u \in \mathcal{V}.$$

If a non-isothermal modeling or gas-quality tracking is considered, further mixing-type constraints need to be incorporated as well; see, e.g., [14, 31].

2.2. **Pipes.** Pipes $a = (u, v) \in \mathcal{A}_{\text{pi}}$ outnumber all other elements in gas networks. Roughly speaking (and ignoring dynamic, thermal, and gravitational effects), gas through pipes flows from higher to larger pressures. At the core of modeling gas flow in pipes are the so-called Euler equations for compressible fluids in cylindrical pipes, which are discussed in more detail in [16]. For stationary considerations, a widely accepted model of gas dynamics in a pipe is given by the so-called Weymouth equation [33]

$$p_u^2 - p_v^2 = \Lambda_a |q_a| q_a, \quad a = (u, v) \in \mathcal{A}_{\text{pi}}, \tag{1}$$

where $\Lambda_a = (16\lambda_a c^2 L_a)/(\pi^2) D_a^5$ mainly models the resistance of the pipe caused by turbulent flow that is due to the rough inner pipe walls. It depends on the friction coefficient λ_a, the speed of sound c, the length L_a, and the diameter D_a of the pipe. For a derivation and more details we refer to the chapter [7] in [18]. As it is the case for all arcs, the mass flow is bounded, i.e., we have

$$q_a^- \leq q_a \leq q_a^+, \quad a \in \mathcal{A}.$$

2.3. **Compressors.** The Weymouth equation (1) can also be read such as gas flow through a pipe leads to a pressure loss. Hence, to transport gas over long distances, one needs to increase the gas pressure from time to time. This is realized in so-called compressor machines, which are either turbo or piston compressors. On a meta level, compressors can be in three different states: they can be (i) active and compress gas to increase its pressure, (ii) closed and thus block the gas flow while decoupling the incident pressures, and they can be (iii) in bypass mode, in which the gas flow bypasses the compressor so that the pressure is not changed. If we denote the pressure increase by the compressor as $\Delta p_a \in [\Delta p_a^-, \Delta p_a^+]$, we can model the three states via

$$
\begin{aligned}
q_a^+ s_a &\geq q_a, && a = (u,v) \in \mathcal{A}_{\mathrm{co}}, && \text{(2a)}\\
q_a^- s_a &\leq q_a, && a = (u,v) \in \mathcal{A}_{\mathrm{co}}, && \text{(2b)}\\
\left(p_v^+ - p_u^- - \Delta p_a^+\right) s_a + p_v - p_u &\leq p_v^+ - p_u^-, && a = (u,v) \in \mathcal{A}_{\mathrm{co}}, && \text{(2c)}\\
\left(p_u^+ - p_v^- + \Delta p_a^-\right) s_a + p_u - p_v &\leq p_u^+ - p_v^-, && a = (u,v) \in \mathcal{A}_{\mathrm{co}}, && \text{(2d)}\\
s_a &\in \{0,1\}, && a = (u,v) \in \mathcal{A}_{\mathrm{co}}, && \text{(2e)}
\end{aligned}
$$

where the binary variable s_a models the compressor being either closed ($s_a = 0$) or open when it is active or in the bypass state ($s_a = 1$); see [11] for more details. Note that the bypass state requires $\Delta p_a^- = 0$. To get a more realistic model of the compression process, so-called characteristic diagrams need to be included in the model that, roughly speaking, couple the ability to increase the gas pressure with the amount of gas flowing through the machine. Incorporating this leads to highly nonlinear constraints

$$
c_{\mathcal{A}_{\mathrm{co}}}(q_a, p_u, p_v, s_a, x_a) \geq 0, \quad a = (u,v) \in \mathcal{A}_{\mathrm{co}},
$$

that also depend on further auxiliary variables x_a that are required to model the characteristic diagrams. For the details we refer to [27], where the modeling of compressor stations is discussed. Compressor stations contain multiple compressor machines that can be combined in combinations of parallel and serial connections, which introduces further combinatorics; see also [11] for details on station modeling.

2.4. **Control Valves and Valves.** Usually, large transport pipelines are operated at high pressure levels with up to more than 100 bar. Such pressure levels can, however, not be used in more regional distribution structures of the network. Hence, control valves $a = (u,v) \in \mathcal{A}_{\mathrm{cv}}$ are used to decrease the gas pressure. They can be modeled using a slight modification of Constraint (2), which then leads to the mixed-integer linear constraints

$$
\begin{aligned}
q_a^+ s_a &\geq q_a, && a = (u,v) \in \mathcal{A}_{\mathrm{cv}},\\
q_a^- s_a &\leq q_a, && a = (u,v) \in \mathcal{A}_{\mathrm{cv}},\\
\left(p_v^+ - p_u^- + \Delta p_a^-\right) s_a + p_v - p_u &\leq p_v^+ - p_u^-, && a = (u,v) \in \mathcal{A}_{\mathrm{cv}},\\
\left(p_u^+ - p_v^- - \Delta p_a^+\right) s_a + p_u - p_v &\leq p_u^+ - p_v^-, && a = (u,v) \in \mathcal{A}_{\mathrm{cv}},\\
s_a &\in \{0,1\}, && a = (u,v) \in \mathcal{A}_{\mathrm{cv}}.
\end{aligned}
$$

Valves are similar elements and can be modeled using two different states. If they are open, they act like control valves in bypass state. If they are closed, the gas flow is blocked and the incident pressures are decoupled. Hence, they can be open (without leading to any pressure loss) or closed (leading to zero flow and decoupled pressures), which can be modeled by the mixed-integer linear constraints

$$
\begin{aligned}
q_a^+ s_a &\geq q_a, && a = (u,v) \in \mathcal{A}_{\mathrm{vl}},\\
q_a^- s_a &\leq q_a, && a = (u,v) \in \mathcal{A}_{\mathrm{vl}},\\
\left(p_v^+ - p_u^-\right) s_a + p_v - p_u &\leq p_v^+ - p_u^-, && a = (u,v) \in \mathcal{A}_{\mathrm{vl}},\\
\left(p_u^+ - p_v^-\right) s_a + p_u - p_v &\leq p_u^+ - p_v^-, && a = (u,v) \in \mathcal{A}_{\mathrm{vl}},\\
s_a &\in \{0,1\}, && a = (u,v) \in \mathcal{A}_{\mathrm{vl}}.
\end{aligned}
$$

2.5. **Objective Functions.** Different objective functions are used in the literature of gas network optimization. The simplest one is a constant objective function, which leads to a pure feasibility problem that asks for a control of compressors, control valves, and valves so that the so-called nomination (the vector of all given supplies q_u, $u \in \mathcal{V}_+$, and withdrawals q_u, $u \in \mathcal{V}_-$) can be transported through the network without violating any physical laws or technical constraints; see, e.g., [25] and the references therein.

Another frequently used objective function minimizes the amount of energy that is required to propel the compressor machines since this represents the largest costs to operate the network.

2.6. **Discussion.** Given the physical as well as technical constraints, the variable bounds, and the objective functions discussed so far, we obtain a highly nonlinear and mixed-integer optimization problem (MINLP). In these models, the number of integer variables is proportional to the number of controllable elements such as compressors, control valves, and valves. Since real-world networks can have more than 4000 nodes and even more arcs, see [29], these MINLPs have to be solved on large graphs, leading to highly challenging instances that often cannot be solved with state-of-the-art general-purpose software. This is the reason why many problem-specific solution methods have been developed over the last decades, which we briefly discuss in the next section.

3. Solution Approaches

Solution approaches for finite-dimensional and mixed-integer nonlinear gas transport problems can be categorized in four groups:

(a) Approaches that solve the MINLP as it is, i.e., without linearizing nonlinearities and without getting rid of integer variables.
(b) MILP-based approaches that use powerful state-of-the-art MILP solvers after the nonlinearities of the model have been appropriately linearized.
(c) NLP-based approaches that focus on the remaining nonlinear problem after the integer variables have been fixed.
(d) MPEC-based approaches that also keep the nonlinearities as they are but that try to reformulate the integer variables with additional continuous variables and constraints.

This categorization is in line with the type of solver that is actually used to solve a specific instance in the end. While approaches in (a) use MINLP solvers, the approaches in (b)–(d) are mainly reformulation techniques so that the reformulated model is finally solved by an MILP, NLP, or MPEC solver.

In what follows, we will briefly discuss the basic aspects of these approaches and give pointers to the literature, where the details can be found. Before we start, let us please mention that the overall body of literature in this area is huge. Due to space limitations, we cannot give a comprehensive overview and we suggest that the interested reader also studies the references cited in the papers that we discuss below.

3.1. **MINLP-Based Approaches.** MINLP-based approaches neither try to get rid of integer variables by continuous reformulations nor do they try to linearize nonlinearities. Instead, they solve the MINLP "as it is". To this end, classic branch-and-bound is typically used for dealing with integer variables and additional spatial branching is required to tackle nonconvex constraints with the help of convex envelopes.[1] However, the combination of discrete aspects as well as nonlinear phenomena makes these MINLPs very hard to solve on large-scale gas transport network instances.

[1] We refrain from citing general literature on MINLP techniques in detail but refer to the survey [3] and the book [19].

Gas-specific MINLP techniques such as problem-tailored convex envelopes, together with suitable spatial branching strategies, have been developed in [25] for the nonlinear Weymouth equation (1). If spatial branching is not used, convex relaxations can be used directly to compute feasible points of good quality as it has been done in [4] for a gas network expansion planning problem, where convex mixed-integer second-order cone relaxations have been developed. Further lower-bounding schemes using tailored relaxations have been in developed [36]. Moreover, tailored MILP and NLP techniques can be used within one search tree for the underlying MINLP as it is done in [17].

3.2. **MILP-Based Approaches.** One key challenge of gas transport MINLPs are the underlying physics that introduce nonlinearities to the problem. Hence, there is a rather large branch of literature that deals with piecewise linear approximations or relaxations of gas-specific nonlinearities that can be solved with state-of-the-art MILP solvers; see, e.g., the seminal papers [5, 23] or the recent tutorial [3]. This approach has the clear advantage in addressing the discrete aspects of the problem but it is often problematic to model arbitrary and particularly higher-dimensional nonlinearities. Moreover, MILP approaches need to introduce additional integer variables for modeling piecewise linear functions, which often leads to large-scale MILPs that are computationally challenging.

Early works include piecewise linear approximation for stationary [24] and time-dependent flows [21]. Moreover, in [8–11], piecewise linear relaxations have been studied.

3.3. **NLP- and MPEC-Based Approaches.** Another branch of research puts the focus on the nonlinearities of the gas transport model at hand. If standard NLP solvers are to be used, almost arbitrary nonlinearities (except for smoothness properties and constraint qualifications) can be considered. However, discrete aspects need to be neglected, which is why many approaches assume them to be given and fixed; see, e.g., [6, 12, 26, 31]. If the NLP is feasible, this leads to an overall feasible point of the underlying MINLP. If not, an iteration needs to be carried out trying other given and fixed discrete variables. For the case of models without integer variables, some research also focuses on time-dependent models and the respective discretizations of the underlying differential equations [15, 32, 37]. Besides the focus on the differential equations, NLP type models are often used to consider highly detailed models of compressors; see, e.g., [22] and [27].

The latter paper also is an example for another strand of research, in which NLP-based models are extended by further, often complementarity, constraints to incorporate discrete aspects in purely continuous models. This leads to so-called mathematical programs with complementarity (or equilibrium) constraints [20], which can be used to model either-or type aspects such as opening or closing compressors or valves; see, e.g., [30]. However, it has also been used to model pooling-type quality mixing aspects [14] or flow direction reversal in pipelines [1, 2].

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