

GAS TRANSPORT NETWORK OPTIMIZATION: PDE-CONSTRAINED MODELS

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1. INTRODUCTION

The optimal control of gas transport networks was and still is a very important topic for modern economies and societies. Accordingly, a lot of research has been carried out on this topic during the last years and decades. Besides mixed-integer aspects in gas transport network optimization, one of the main challenges is that a physically and technically detailed modeling of transient gas dynamics leads to theoretically and computationally highly demanding models involving nonlinear partial differential equations (PDEs). For further background on the application, historical notes and a detailed discussion of mixed-integer aspects for stationary descriptions we refer to Hante and Schmidt [18]. In this chapter, we focus on the most common modeling approaches concerning transient descriptions, point out the challenges, and summarize important contributions concerning the optimization of the most relevant control parameters for this particular class of problems.

2. PIPE MODELING

For modeling gas networks, a key modeling decision concerns the governing equations for the gas flow in pipes. Long sections of cylindrical pipes are commonly modeled as one-dimensional objects parameterized in length from inlet to outlet by the spatial variable $x \in [0, L]$, featuring a (constant) diameter D and a height-profile $h : [0, L] \rightarrow \mathbb{R}$. As a compressible fluid, the gas flow through the pipe under the assumption of a constant temperature T is then described in terms of density ρ , velocity v , and pressure p with the governing equations

$$\begin{aligned}\partial_t \rho + \partial_x(\rho v) &= 0, \\ \partial_t(\rho v) + \partial_x(p + \rho v^2) &= -\frac{\lambda}{2D} \rho v |v| - g \rho h',\end{aligned}\tag{1}$$

together with the constitutive law

$$p = R_s \rho T z(p, T),$$

where g models gravitational forces, λ is the friction factor of the pipe's inner wall, and where R_s denotes the specific gas constant and $z(p, T)$ the compression factor for the underlying gas composition [3, 29, 36]. The dependency of $z(p, T)$ on p and T is often approximated by empirically derived models, e.g., by the AGA [27] or the Papay [33] formula.

These equations yield a system of nonlinear and hyperbolic balance laws with two characteristics $\lambda_1 = v - c$ and $\lambda_2 = v + c$, where c is the speed of sound within the gas given by $c^2 = \partial_\rho p$. They are often considered in the variables of gas pressure p and of mass flow $q = A \rho v$ with the pipe's cross-sectional area $A = \pi D^2/4$.

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Most optimal control problems concern subsonic regimes $|v| \ll c$. An often used simplification concerns the idealization $z(p, T) \equiv \text{const}$. The neglect of the ram pressure term ρv^2 on the left-hand side in (1) then yields the semilinear model

$$\begin{aligned} \partial_t p + \frac{c^2}{A} \partial_x q &= 0, \\ \partial_t q + A \partial_x p &= -\frac{\lambda c^2}{2DA} \frac{q|q|}{p} - \frac{gA}{c^2} h' p. \end{aligned} \quad (2)$$

Dropping $\partial_t q$ in (2) leads to the quasi-stationary (so-called friction dominated) model

$$\begin{aligned} \partial_t p + \frac{c^2}{A} \partial_x q &= 0, \\ A \partial_x p &= -\frac{\lambda c^2}{2DA} \frac{q|q|}{p} - \frac{gA}{c^2} h' p. \end{aligned} \quad (3)$$

Dropping all time derivatives in (2) yields $q \equiv \text{const}$ and, when further neglecting the gravity term, one obtains the so-called Weymouth equation

$$p_{\text{in}}^2 - p_{\text{out}}^2 = \frac{\lambda c^2 L}{DA^2} q |q|$$

for the pressure at the in- and outlet of the pipe often used for a stationary modeling; see [18]. The relevant pipe model depends on the specific application and desired (modeling) accuracy. This isothermal model hierarchy also extends to temperature-dependent models and port-Hamiltonian descriptions are available as well. For further details see [3, 4].

For well-posedness, the dynamic gas flow pipe models are to be complemented with initial conditions, e.g., at $t = 0$ via

$$p(0, x) = p_0(x), \quad q(0, x) = q_0(x), \quad x \in [0, L].$$

Moreover, when transmission or boundary conditions for p and/or q at the in- and/or outlet are prescribed, they have to respect the characteristics of the chosen flow model in the strong or corresponding weak form of these equations. For a single pipe, typically either p or q is prescribed at both in- and outlet.

3. NETWORK MODELING

The dynamics of a gas network over a time period $[0, \mathcal{T}]$ is modeled using a directed graph $G = (\mathcal{V}, \mathcal{A})$ with node set \mathcal{V} and arc set \mathcal{A} . For transient descriptions arcs $a \in \mathcal{A}$ are associated with pipes of length L_a ; with pressures p_a and flows q_a being governed by either (1), (2), or (3). The nodes $u \in \mathcal{V}$ model junctions, boundary nodes, or active elements such as compressors, valves, and the like by prescribing additional algebraic conditions using $\delta^{\text{in}}(u)$ and $\delta^{\text{out}}(u)$ for the set of in- and outgoing arcs.

Typical junction conditions are the continuity of pressure, i.e.,

$$\begin{aligned} p_a(t, 0) &= p_u(t) \quad \text{for all } a \in \delta^{\text{out}}(u), \\ p_a(t, L_a) &= p_u(t) \quad \text{for all } a \in \delta^{\text{in}}(u), \end{aligned} \quad (4)$$

for some function $p_u(t)$, which can be interpreted as the pressure at that node at time t , and the balance of flows, i.e.,

$$\sum_{a \in \delta^{\text{out}}(u)} q_a(t, 0) - \sum_{a \in \delta^{\text{in}}(u)} q_a(t, L_a) = q_u(t), \quad t \in [0, \mathcal{T}], \quad (5)$$

where $q_u(t)$ is an in- or outflow at that node at time t .

Boundary nodes are in many cases required to have edge degree 1 and typically prescribe either pressure or flow on the respective end of its incident arc via (4)

or (5) as a boundary condition for the associated pipe. The values $p_u(t)$ or $q_u(t)$ are sometimes considered as a control $w_u(t)$ of the system.

Nodes u modeling active elements are usually required to have exactly one in- and one outgoing arc $(a_{\text{in}}, a_{\text{out}})$ and impose certain parameter-dependent linear or nonlinear coupling conditions for the pressure or flow across the node. For instance, for u in a subset $\mathcal{V}_c \subset \mathcal{V}$ modeling compressors, one can use the model

$$q_{a_{\text{out}}}(t, 0) = q_{a_{\text{in}}}(t, L_{a_{\text{in}}}), \quad p_{a_{\text{out}}}(t, 0) = p_{a_{\text{in}}}(t, L_{a_{\text{in}}}) \exp\left(\frac{w_u(t)}{q_{a_{\text{out}}}(t, 0)}\right), \quad t \in [0, \mathcal{T}],$$

where $w_u(t)$ is proportional to the energy of the compression process [1]. The value $w_u(t)$ is often also considered as a control. More detailed models of compressor machines as well as transient models for (control) valves, resistors, and the like are presented in [4]. Sometimes, active elements such as compressors are also placed on special (non-pipe) arcs [2], as it is common for stationary modeling [18].

All controls are typically bounded from below and above via

$$w_u^-(t) \leq w_u(t) \leq w_u^+(t), \quad t \in [0, \mathcal{T}],$$

with given $w_u^\pm(t)$. Certain control parameters may also be required to be binary- or integer-valued to model opening/closing of valves or more complex routing options within compressor stations consisting of several machines [14, 16, 24]. Moreover, within the network, pressures are often required to also obey bounds such as

$$p_a^- \leq p_a(t, x) \leq p_a^+, \quad (t, x) \in [0, \mathcal{T}] \times [0, L_a], \quad a \in \mathcal{A},$$

with typically constant and given values p_a^\pm . Similar restrictions may apply for flows at the boundary nodes as to model, e.g., certain minimal or maximal demands.

Classic objective functions then consist of a sum of tracking-type objectives eventually combined with standard control regularization terms such as of Tikhonov-type [8, 16]. Usual goals are to steer the system as close as possible to a desired network state, e.g., close to stationary, to minimize a specific demand gap, or to minimize the necessary compression power, e.g., in the sense that [1]

$$\sum_{u \in \mathcal{V}_c} \int_0^{\mathcal{T}} \|w_u(t)\|^2 dt \rightarrow \min,$$

while respecting all governing equations and all bounds. The resulting problems then belong to the class of state-constrained optimal control problems for nonlinear PDEs.

4. CONTRIBUTIONS IN THE FIELD

When the modeling presented in Sections 2 and 3 is applied to a real-world gas network with hundreds or thousands of pipes, the resulting problems are large-scale dynamical optimization problems. In this case, already the evaluation of the network state for a fixed control using numerical methods is a challenging task [2]. Any optimization approach therefore needs to balance accuracy and tractability. The important issue thereby is to handle the nonlinear pressure-drop term in the right-hand side of (1), (2), or (3) appropriately. Often, additional simplifications such as assumptions on network sizes or certain network topologies are made. Whenever transient models are employed, the time horizons under considerations are also typically short. Many available studies concern so-called day-ahead operation, which is then applied in a receding or moving horizon fashion [34]. For approaches based on mathematical optimization, an important distinction is whether the problem is either first discretized in order to directly apply methods from finite-dimensional nonlinear optimization or to tackle the problem indirectly using suitable reformulations as to

apply tailored infinite-dimensional optimality conditions from the field of optimal control and to then solve these numerically using discretizations.

4.1. Direct Methods. In these approaches, all governing equations are first replaced by finite-dimensional approximations and are subsequently solved using methods from nonlinear optimization. A majority of work is based on methods from classic nonlinear optimization but differs in the used methods for discretization, for the computation of gradients, and the specific algorithms used to compute stationary points:

- Standard sequential quadratic programming can be applied to (adaptive) implicit box-schemes, where gradients are computed using a discrete adjoint approach [5];
- Standard interior-point methods can be applied to pseudospectral collocation methods, where gradients then come in sparse form [42]. Such approaches can also incorporate uncertainties using a two-stage stochastic programming method [41];
- The structure of Euler discretizations can also be exploited in tailored primal-dual interior-point solvers [37];
- Gradient information for certain discretizations can also be obtained from formal adjoint approaches [19, 22].

Alternatively, after discretization, different reformulations can be used to apply other, also non-local, methods from mathematical optimization. This includes mixed-integer linear optimization, where nonlinearities are approximated by piecewise linear functions [31], or instantaneous control approaches, where tailored mixed implicit-explicit Euler discretization yield linear constraints for every time-step [11]. A similar approach is followed in [24], using approximations leading to linear constraints over several time steps and incorporating this into a moving-horizon scheme. Further global approaches are simulated annealing [32] or, for simple network topologies, dynamic programming [40].

Most of these approaches are capable to provide reasonable solutions on small-to medium-size benchmark problems such as available in [2] and some even proved success on real networks.

4.2. Theory for Indirect Approaches. A particular focus for PDE-constrained gas network optimization problems is on developing adequate indirect solution approaches. They heavily rely on regularity properties of the underlying control-to-state map, its gradient representations using adjoint equations, and an appropriate treatment of both integer and state constraints in order to obtain suitable optimality conditions and their discretizations. Standard methods from PDE-constrained optimization [23, 30, 38] cannot be apply directly due to the heterogeneous domain of functions on graphs, the hyperbolic character of (1)–(2), the nonlinearities in (1)–(3), and the coupling conditions (4)–(5). Key contributions concern the following:

- Existence and regularity of solutions [1, 12, 13] and structural analysis such as steady-state characterizations and stabilization [9, 10], controllability [6], as well as turnpike properties [8];
- Adjoint calculus, e.g., for classical solutions of hyperbolic systems based on Riemann invariants [7] or for entropy solutions of balance laws [35];
- State-constraint handling by Moreau–Yosida type regularizations [21, 35];
- Optimality conditions obtained using linearization [8] or parabolic regularization [20]. These can then be solved using semismooth Newton-methods [39];
- Domain decomposition techniques as to keep larger systems or longer time horizons tractable [25, 26, 28];

- Mixed-integer control handling using relaxation and combinatorial integral approximation [14, 15, 17].

Most of these techniques were already be successfully applied to academic problems motivated from PDE-constrained gas network problems.

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