Chapter 9

An MPEC based heuristic

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Abstract *In this chapter we discuss the problem of validation of nominations as a nonsmooth and nonconvex mixed-integer nonlinear feasibility problem. For this problem we present a primal heuristic that is based on reformulation techniques that smooth the appearing nonsmooth aspects and that reformulate discrete aspects with complementarity constraints and problem specific relaxations. The resulting mathematical program with equilibrium constraints (MPEC) model can be regularized by standard techniques leading to a nonlinear program (NLP) type model. Solutions to the latter can finally be used as approximative solutions to the underlying feasibility problem.*

In this chapter, we review the problem of validation of nominations as a *nonsmooth mixed-integer nonlinear feasibility problem* and develop a problem-specific primal heuristic. In contrast to other approaches like the ones described in Chapter 6 or 7, we explicitly distinguish between

1. discontinuous aspects including discrete decisions leading to mixed-integer formulations using binary variables and
2. nonsmooth, but continuous aspects.

Since our aim is to employ standard solvers for (smooth) nonlinear optimization, we *reformulate* both the integer and the nonsmooth aspects. It will turn out that most of the integer parts of the validation of nominations model can be exactly reformulated by using complementarity constraints leading to a mathematical program with equilibrium constraints (MPEC). This model type is a generalization of nonlinear programs (NLPs) in which so-called *equilibrium* or *complementarity constraints* of the form

$$\phi_i(x)\psi_i(x) = 0, \quad \phi_i(x) \geq 0, \quad \psi_i(x) \geq 0, \quad i = 1, \ldots, k, \tag{9.1}$$

appear, where $\phi_i, \psi_i : \mathbb{R}^n \to \mathbb{R}$ are smooth functions. See Luo, Pang, and Ralph (1996) for an overview of MPECs. The remaining nonsmooth parts are *smoothed* by applying both standard and problem-specific smoothing techniques. The resulting smooth MPEC has the well-known drawback that it lacks standard constraint qualifications (CQs) like LICQ or MFCQ (see Ye and Zhu (1995)). Since these CQs are a major assumption for the convergence theory of almost every NLP solver, there is no convergence theory when

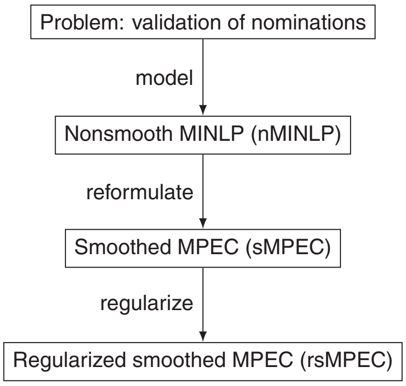

Figure 9.1. *Relationship of models studied in this chapter.*

applying standard NLP solvers directly to mathematical program with equilibrium constraintss (MPECs). Because we want to use standard NLP solvers for our primal heuristic, we finally have to *regularize* the MPEC to get an NLP satisfying standard CQs. The description and analysis of some standard regularization schemes for MPECs can be found in Scholtes (2001), DeMiguel et al. (2005), and Hu and Ralph (2004). Here we use a penalization scheme that regularizes the MPEC by moving the complementarity constraints (9.1) to the objective function. The details will be discussed later. Summarizing, we get a hierarchy of model formulations. An overview is given in Figure 9.1.

One central goal of our heuristic approach is that it should produce feasible solutions of the underlying nonsmooth mixed-integer nonlinear program (nMINLP) for real-world instances in a short time. Thus, it is not reasonable to incorporate all gas physics and engineering aspects. On the other hand, we have to incorporate as many physics and engineering details as necessary such that the consecutive NLP validation (see Chapter 10) has a high rate of positive validations. Thus, we performed numerical experiments that led us to the following modeling decisions:

1. We neglect all composition-specific gas parameters and the corresponding mixing model. The gas parameters appearing in the constraints of our model are mean values in dependence of the network data and the concrete nomination.
2. We only consider the isothermal case, i.e., the gas temperature is assumed to be constant. Thus, we can neglect all constraints concerning heat dynamics.
3. We disregard small pressure losses in control valve stations and compressor groups, which are caused by inner station piping, flow through measuring systems, or filters; see Chapter 2. Thus, we neglect up- and downstream resistors (see Chapter 10) that are used to model these potential pressure losses. In contrast, we account for resistors located outside of control valve stations and compressor groups.
4. We incorporate the highly nonlinear and nonconvex models of the operating ranges of compressor machines (see Section 2.3.5) without any further simplifications.

The chapter is organized as follows. In Section 9.1 we give a formulation of the problem of validation of nominations as an nMINLP. In addition, we directly develop the MPEC based reformulations of the mixed-integer parts and describe the smoothing techniques applied to nonsmooth aspects. The section ends with a complete description of both nMINLP as well as its smoothed and MPEC based reformulation sMPEC. Afterwards, Section 9.2 describes the used regularization scheme for MPECs that enables us to apply standard NLP solvers for solving the final problem formulation rsMPEC. Since the resulting regularized MPEC is extremely hard to solve for current solvers, we split up the solution process into two stages that are described in Section 9.3.

9.1 ▪ Model

In this section, we present a nonsmooth mixed-integer nonlinear model of every component of the gas transport networks under consideration (see Chapter 2). Based on this model, we develop reformulations using smoothing techniques and complementarity constraints that are used to finally build up the NLP based primal heuristic. The reader interested in a more detailed description of the used reformulation techniques can find additional information in Schmidt (2013) and Schmidt, Steinbach, and Willert (2013). A related model of natural gas transport using complementarity constraints was recently published by Baumrucker and Biegler (2010). These authors use MPEC techniques for handling nonsmooth model aspects like flow reversals and flow state transitions. In contrast, we use problem-specific smoothing techniques for these aspects and apply MPEC techniques for modeling the discrete control of active elements.

For ease of notation, the nonsmooth mixed-integer nonlinear program (nMINLP) model is stated in standard NLP form,

$$\min_{x \in \mathscr{X}} \quad f(x) \quad \text{s.t.} \quad c_{\mathscr{E}}(x) = 0, \quad c_{\mathscr{I}}(x) \geq 0,$$

and will be discussed componentwise in the following sections. The decision vector $x \in \mathscr{X} := \mathbb{R}^n \times \{0,1\}^m$ consists of real and binary variables. A subindex refers to the sub-vector of the corresponding network element or set of elements. For instance, x_u denotes the variables of the component model of node u, and $x_{A_{\text{pi}}}$ denotes the variables of the component models of all pipes. Single constraints $c : \mathscr{X} \to \mathbb{R}$ are subindexed with the corresponding vertex u or arc a and superindexed with an abbreviated name describing the semantics of the constraint. For instance, c_u^{flow} is the constraint modeling the flow balance at node u. Complete component models are written as vectors of constraints $c : \mathscr{X} \to \mathbb{R}^k$, with subindices indicating single elements or sets thereof, as for the variables. If necessary, a subindex $\mathscr{E}$ or $\mathscr{I}$ is used to distinguish between equality and inequality constraints. Finally, objective functions or portions thereof are denoted by f.

9.1.1 ▪ Nodes

Nodes $u \in V$ are modeled as elements without capacity, satisfying the mass balance equation (see (2.8))

$$0 = c_u^{\text{flow}}(x) = \sum_{a \in \delta^+(u)} q_a - \sum_{a \in \delta^-(u)} q_a - q_u^{\text{nom}}, \tag{9.2}$$

where q_a is the mass flow on arc a and $q^{\text{nom}} \in \mathbb{R}^V$ is the flow supply/demand vector:

$$\begin{aligned} q_u^{\text{nom}} &\geq 0, \quad u \in V_+ \quad \text{(entries)}, \\ q_u^{\text{nom}} &= 0, \quad u \in V_0 \quad \text{(inner nodes)}, \\ q_u^{\text{nom}} &\leq 0, \quad u \in V_- \quad \text{(exits)}. \end{aligned}$$

In addition, every node u has a gas pressure variable p_u with bounds $[\underline{p}_u, \overline{p}_u]$ that depend on technical and/or contractual data. The complete node model reads

$$0 = c_u(x) = c_u^{\text{flow}}(x), \quad x_u = p_u.$$

It does not require any reformulation.

9.1.2 ▪ Pipes

A pipe $a = (u, v) \in A_{\text{pi}}$ generally requires a complicated PDE model describing the gas dynamics in terms of mass, momentum, and energy balances: the Euler equations for compressible fluids (see Feistauer (1993); Lurie (2008); Schmidt, Steinbach, and Willert (2014)). These equations and all other relevant basics of the fluid model can be found in Section 2.3.1. For the ease of understanding, we use the same notation as in Section 2.3.1. For the isothermal and stationary case considered here, the mass balance (continuity equation) yields constant mass flow q along the pipe, the energy equation is not needed, and we are left with a stationary variant of the *momentum equation*; see (2.13). The state quantities pressure p, density ρ and temperature T (constant in our case) are coupled by an *equation of state*; we use the thermodynamical standard equation

$$\rho = \rho(p, T) = \frac{p}{R_{\text{s}} z(p, T) T},$$

where R_{s} is the specific gas constant; see (2.20). Finally, we need empirical models for the *compressibility factor* $z(p, T)$, describing the deviation of real gas from ideal gas, and for the *friction coefficient* $\lambda(q)$. The latter will be discussed later; for the former we use the AGA formula (2.5). For details and alternative models see Chapter 2 or Schmidt, Steinbach, and Willert (2014).

The stationary momentum equation essentially yields the pressure loss along the pipe for which various approximation formulas exist; see Saleh (2002) or Schmidt, Steinbach, and Willert (2014). Here we use a quadratic equation of Weymouth type (see Katz (1959); Weymouth (1912); de Nevers (1970)) derived in Lurie (2008),

$$0 = c_a^{\text{p-loss}}(x) = p_v^2 - \left(p_u^2 - \Lambda_a q_a |q_a| \frac{e^{S_a} - 1}{S_a} \right) e^{-S_a}, \tag{9.3}$$

where

$$\Lambda_a = \frac{L_a}{A_a^2 D_a} z_{a,\text{m}} T R_{\text{s}} \lambda_a, \quad S_a = \frac{2 L_a g s_a}{R_{\text{s}} z_{a,\text{m}} T}.$$

The used quantities are the length of the pipe L_a, the constant slope of the pipe s_a, its cross-sectional area A_a and its diameter D_a. The gravitational acceleration is denoted by g. See Section 2.3.1.2 for the details. Both coefficients Λ_a and S_a depend on p_u, p_v via $z_{a,\text{m}}$ and $p_{a,\text{m}}$: we use approximate mean values of the compressibility factor and pressure defined by

$$0 = c_a^{\text{p-mean}}(x) = p_{a,\text{m}} - \frac{2}{3} \left(p_u + p_v - \frac{p_u p_v}{p_u + p_v} \right),$$
$$0 = c_a^{\text{z-mean}}(x) = z_{a,\text{m}} - z(p_{a,\text{m}}, T).$$

Finally, we model the friction coefficient $\lambda(q)$ by the Hagen–Poiseuille formula for laminar flow (2.16),

$$\lambda^{\text{HP}}(q) = \frac{64}{Re(q)}, \quad q \le q_{\text{crit}},$$

and by the implicit empirical model of Prandtl–Colebrook (2.17) for turbulent flow,

$$\frac{1}{\sqrt{\lambda^{\text{PC}}(q)}} = -2 \log_{10} \left(\frac{2.51}{Re(q) \sqrt{\lambda^{\text{PC}}(q)}} + \frac{k}{3.71 D} \right), \quad q > q_{\text{crit}}.$$

Here, k is the roughness of the inner pipe wall and Re is the Reynolds number. If we replace the variable λ_a in $c_a^{\text{p-loss}}$ (9.3) with the new variable λ_a^{HPPC} subject to the nonsmooth constraint

$$0 = c_a^{\text{HPPC}}(x) = \lambda_a^{\text{HPPC}} - \begin{cases} \lambda^{\text{HP}}(q_a), & q_a \le q_{\text{crit}}, \\ \lambda^{\text{PC}}(q_a), & q_a > q_{\text{crit}}, \end{cases} \tag{9.4}$$

we end up with the nonsmooth pipe model

$$0 = c_a(x) = \begin{pmatrix} c_a^{\text{p-loss}}(x) \\ c_a^{\text{p-mean}}(x) \\ c_a^{\text{z-mean}}(x) \\ c_a^{\text{HPPC}}(x) \end{pmatrix}, \quad x_a = \begin{pmatrix} q_a \\ z_{a,\text{m}} \\ p_{a,\text{m}} \\ \lambda_a^{\text{HPPC}} \end{pmatrix}. \tag{9.5}$$

Pipe model reformulation: Smoothing The pipe model (9.5) is discontinuous at $q_a = q_{\text{crit}}$ due to c_a^{HPPC} (9.4) and second-order discontinuous at $q_a = 0$ due to the term $q_a|q_a|$ in $c_a^{\text{p-loss}}$ (9.3). We address both difficulties simultaneously by replacing $\Lambda_a q_a |q_a|$ in (9.3) by $\tilde{\Lambda}_a \phi_a$:

$$0 = c_a^{\text{p-loss-s}}(x) = p_v^2 - \left(p_u^2 - \tilde{\Lambda}_a \phi_a \frac{e^{S_a} - 1}{S_a} \right) e^{-S_a},$$

where $\tilde{\Lambda}_a := \Lambda_a / \lambda_a$ and ϕ_a approximates the term $\lambda_a^{\text{HPPC}} q_a |q_a|$,

$$0 = c_a^{\text{HPPC-s}}(x) = \phi_a - r_a \left(\sqrt{q_a^2 + e_a^2} + b_a + \frac{c_a}{\sqrt{q_a^2 + d_a^2}} \right) q_a.$$

This smoothing has been shown to provide an asymptotically correct second-order approximation of $\lambda_a^{\text{HPPC}} q_a |q_a|$ if $e_a, d_a > 0$ and

$$r_a = (2 \log_{10} \beta_a)^{-2}, \quad b_a = 2\delta_a, \quad c_a = (\ln \beta_a + 1)\delta_a^2 - \frac{e_a^2}{2},$$

with

$$\alpha_a = \frac{2.51 A_a \eta}{D_a}, \quad \beta_a = \frac{k_a}{3.71 D_a}, \quad \delta_a = \frac{2\alpha_a}{\beta_a \ln 10},$$

(see Burgschweiger, Gnädig, and Steinbach (2009); Schmidt, Steinbach, and Willert (2014)). Here, η is the dynamic viscosity of the gas which we assume to be a constant; see Section 2.3.1. In summary, we obtain the smooth pipe model

$$0 = c_a^{\text{smooth}}(x) = \begin{pmatrix} c_a^{\text{p-loss-s}}(x) \\ c_a^{\text{p-mean}}(x) \\ c_a^{\text{z-mean}}(x) \\ c_a^{\text{HPPC-s}}(x) \end{pmatrix}, \quad x_a^{\text{smooth}} = \begin{pmatrix} q_a \\ z_{a,\text{m}} \\ p_{a,\text{m}} \\ \phi_a \end{pmatrix}.$$

9.1.3 ▪ Resistors

A resistor $a = (u, v) \in A_{\text{rs}}$ is a fictitious network element modeling the approximate pressure loss across gadgets, partly closed valves, filters etc.; see also Section 2.3.2. The pressure loss has the same sign as the mass flow and is either assumed to be (piecewise) constant,

$$0 = c_a^{\text{p-loss-lin}}(x) = p_u - p_v - \zeta_a \operatorname{sgn}(q_a), \tag{9.6}$$

or (piecewise) quadratic according to the law of Darcy–Weisbach (see Lurie (2008); Finnemore and Franzini (2002)),

$$0 = c_a^{\text{p-loss-nl}}(x) = p_u - p_v - \frac{8\zeta_a}{\pi^2 D_a^4} \frac{q_a |q_a|}{\rho_{a,w}}. \tag{9.7}$$

Here $\zeta_a \geq 0$ is the resistance coefficient, and $\rho_{a,w}$ is the inflow gas density, which is determined via

$$0 = c_a^{\text{dens-in}}(x) = \rho_{a,w} - \rho(p_w, T) \quad \text{with} \quad w := \begin{cases} u, & q_a \geq 0, \\ v, & q_a < 0. \end{cases} \tag{9.8}$$

The compressibility factor z has to be evaluated at the inflow node as well,

$$0 = c_a^{\text{z-in}}(x) = z_{a,w} - z(p_w, T).$$

In summary, the piecewise constant resistor model ($a \in A_{\text{lin-rs}}$) reads

$$0 = c_a(x) = c_a^{\text{p-loss-lin}}(x), \quad x_a = q_a, \tag{9.9}$$

and the piecewise quadratic resistor model ($a \in A_{\text{nl-rs}}$) reads

$$0 = c_a(x) = \begin{pmatrix} c_a^{\text{p-loss-nl}}(x) \\ c_a^{\text{dens-in}}(x) \\ c_a^{\text{z-in}}(x) \end{pmatrix}, \quad x_a = \begin{pmatrix} q_a \\ z_{a,w} \\ \rho_{a,w} \end{pmatrix}. \tag{9.10}$$

Resistor model reformulation: Smoothing The presented resistor models (9.9) and (9.10) are nonsmooth, because of three reasons:

1. the discontinuous sgn function in (9.6),
2. the second-order discontinuous term $|q_a|q_a$ in (9.7), and
3. the direction dependence of the inflow gas density $\rho_{a,k}$ in (9.7).

In the piecewise constant resistor model, we smooth the sgn function via

$$\text{sgn}(x) = \frac{x}{|x|} = \frac{x}{\sqrt{x^2}} \approx \frac{x}{\sqrt{x^2 + \varepsilon_a}}, \tag{9.11}$$

with a smoothing parameter $\varepsilon_a > 0$. For $a \in A_{\text{lin-rs}}$ this yields

$$0 = c_a^{\text{smooth}}(x) = c_a^{\text{p-loss-lin-s}}(x),$$

with

$$0 = c_a^{\text{p-loss-lin-s}}(x) = p_u - p_v - \zeta_a \frac{q_a}{\sqrt{q_a^2 + \varepsilon_a}}.$$

The same approximation of the absolute value function as in (9.11) is applied to the piecewise quadratic resistor model (9.7):

$$0 = c_a^{\text{p-loss-nl-s}}(x) = p_u - p_v - \frac{8\zeta_a}{\pi^2 D_a^4} \frac{q_a \sqrt{q_a^2 + \varepsilon_a}}{\rho_{a,\text{m}}}.$$

Finally, the direction dependence of the inflow gas density $\rho_{a,k}$ is approximatively addressed by using the mean density

$$0 = c_a^{\text{dens-mean}}(x) = \rho_{a,\text{m}} - \frac{1}{2}\left(\rho_{a,\text{in}} + \rho_{a,\text{out}}\right).$$

As a consequence, we need to evaluate the equation of state and the compressibility factor at both nodes u and v,

$$0 = c_a^{\text{dens-in}}(x) = \rho_{a,\text{in}} - \rho(p_u, T), \qquad 0 = c_a^{\text{dens-out}}(x) = \rho_{a,\text{out}} - \rho(p_v, T),$$
$$0 = c_a^{\text{z-in}}(x) = z_{a,\text{in}} - z(p_u, T), \qquad 0 = c_a^{\text{z-out}}(x) = z_{a,\text{out}} - z(p_v, T).$$

This yields for $a \in A_{\text{nl-rs}}$ the smoothed model

$$0 = c_a^{\text{smooth}}(x) = \begin{pmatrix} c_a^{\text{p-loss-nl-s}}(x) \\ c_a^{\text{dens-in}}(x) \\ c_a^{\text{dens-out}}(x) \\ c_a^{\text{dens-mean}}(x) \\ c_a^{\text{z-in}}(x) \\ c_a^{\text{z-out}}(x) \end{pmatrix}, \quad x_a^{\text{smooth}} = \begin{pmatrix} q_a \\ \rho_{a,\text{in}} \\ \rho_{a,\text{out}} \\ \rho_{a,\text{m}} \\ z_{a,\text{in}} \\ z_{a,\text{out}} \end{pmatrix}.$$

9.1.4 ▪ Short cuts

A short cut $a = (u, v) \in A_{\text{sc}}$ is a fictitious network element involving only a simple pressure equality:

$$0 = c_a^{\text{p-coupl}}(x) = p_u - p_v.$$

Thus, we have the model

$$0 = c_a(x) = c_a^{\text{p-coupl}}(x), \quad x_a = q_a.$$

No reformulation is required.

9.1.5 ▪ Valves

A valve $a = (u, v) \in A_{\text{va}}$ has two discrete states: *open* and *closed*. Across open valves, the pressures are identical and the flow is arbitrary within its technical bounds; see (2.33)–(2.35),

$$p_v = p_u, \quad q_a \in [\underline{q}_a, \overline{q}_a]. \tag{9.12}$$

Closed valves block the gas flow and the pressures are arbitrary within their bounds; see (2.36),

$$q_a = 0, \quad p_u \in [\underline{p}_u, \overline{p}_u], \quad p_v \in [\underline{p}_v, \overline{p}_v]. \tag{9.13}$$

This behavior can be modeled with one binary variable $s_a \in \{0, 1\}$ together with big-M constraints:

$$0 \le c_a^{\text{flow-lb}}(x) = q_a - s_a \underline{q}_a,$$
$$0 \le c_a^{\text{flow-ub}}(x) = -q_a + s_a \overline{q}_a,$$
$$0 \le c_a^{\text{p-coupl-1}}(x) = M_{a,1}(1 - s_a) - p_v + p_u,$$
$$0 \le c_a^{\text{p-coupl-2}}(x) = M_{a,2}(1 - s_a) - p_u + p_v.$$

Here and in what follows, the big M's are chosen sufficiently large in order to deactivate the constraint in case of $s_a = 0$. In the concrete case above, the smallest possible values are $M_{a,1} = \overline{p}_v - \underline{p}_u$ and $M_{a,2} = \overline{p}_u - \underline{p}_v$. The resulting valve model reads

$$0 \le c_a(x) = \begin{pmatrix} c_a^{\text{flow-lb}}(x) \\ c_a^{\text{flow-ub}}(x) \\ c_a^{\text{p-coupl-1}}(x) \\ c_a^{\text{p-coupl-2}}(x) \end{pmatrix}, \quad x_a = \begin{pmatrix} q_a \\ s_a \end{pmatrix}.$$

Valve model reformulation: Complementarity constraints It is easily seen that the switching between *open* and *closed* valve states can be formulated equivalently with the complementarity constraint

$$0 = c_a^{\text{state}}(x) = (p_u - p_v)q_a.$$

Note that this is only possible because the two states are not *disjoint*: there exist triples (q_a, p_u, p_v) that satisfy both (9.12) and (9.13). The complete reformulation reads

$$0 = c_a^{\text{mpec}}(x) = c_a^{\text{state}}(x), \quad x_a^{\text{mpec}} = q_a.$$

It offers two advantages: no binary variables are required and the number of constraints reduces from four to one. The drawback is the loss of model regularity in terms of constraint qualifications.

9.1.6 ▪ Control valves

A control valve $a = (u, v) \in A_{\text{cv}}$ is used to decrease the gas pressure in a technically prescribed direction which is given implicitly by the direction of the arc a. It possesses three discrete states: *active*, *bypass*, and *closed*. An *active* control valve reduces the inflow pressure by a certain amount (see (2.37)),

$$p_v = p_u - \Delta_a, \quad \Delta_a \in [\underline{\Delta}_a, \overline{\Delta}_a], \quad q_a \in [\underline{q}_a, \overline{q}_a] \cap \mathbb{R}_{\geq 0}.$$

A *closed* control valve acts like a closed regular valve, leading to the simple state model (9.13). A control valve in *bypass* mode acts like an open regular valve, with arbitrary flow direction and without decreasing the pressure, see (9.12). Our complete mixed-integer linear model is based on the variable vector

$$x_a = \begin{pmatrix} q_a \\ s_{a,1} \\ s_{a,2} \end{pmatrix},$$

where $s_{a,1}, s_{a,2} \in \{0, 1\}$ have the following interpretation:

$$s_{a,1} = \begin{cases} 0, & a \text{ is closed,} \\ 1, & a \text{ is open,} \end{cases} \qquad s_{a,2} = \begin{cases} 0, & a \text{ is inactive,} \\ 1, & a \text{ is active.} \end{cases}$$

The three states given above are represented as the following combinations:

$$\begin{aligned} (s_{a,1}, s_{a,2}) &= (0, 0)\text{: } a \text{ is closed,} \\ (s_{a,1}, s_{a,2}) &= (1, 0)\text{: } a \text{ is in bypass mode,} \\ (s_{a,1}, s_{a,2}) &= (1, 1)\text{: } a \text{ is active.} \end{aligned}$$

In terms of the constraints

$$\begin{aligned} 0 &\leq c_a^{\text{flow-lb-open}}(x) = q_a - s_{a,1}\underline{q}_a, \\ 0 &\leq c_a^{\text{flow-ub-open}}(x) = -q_a + s_{a,1}\overline{q}_a, \\ 0 &\leq c_a^{\text{flow-lb-active}}(x) = q_a - (1 - s_{a,2})\underline{q}_a, \\ 0 &\leq c_a^{\text{p-coupl-1}}(x) = M_{a,1}(1 - s_{a,1}) + \overline{\Delta}_a s_{a,2} - (p_u - p_v), \\ 0 &\leq c_a^{\text{p-coupl-2}}(x) = M_{a,2}(1 - s_{a,1}) - \underline{\Delta}_a s_{a,2} - (p_v - p_u), \\ 0 &\leq c_a^{\text{consistent-states}}(x) = s_{a,1} - s_{a,2}, \end{aligned}$$

the resulting mixed-integer model then becomes

$$0 \leq c_a(x) = \begin{pmatrix} c_a^{\text{flow-lb-open}}(x) \\ c_a^{\text{flow-ub-open}}(x) \\ c_a^{\text{flow-lb-active}}(x) \\ c_a^{\text{p-coupl-1}}(x) \\ c_a^{\text{p-coupl-2}}(x) \\ c_a^{\text{consistent-states}}(x) \end{pmatrix}. \tag{9.14}$$

Control valve model reformulation: Complementarity constraints As for valves, the reformulation here is based on a complementarity constraint:

$$0 = c_a^{\text{state}}(x) = (p_v - p_u + \Delta_a) q_a.$$

In addition, the restriction to nonnegative flows in the active state is modeled as

$$0 \leq c_a^{\text{active-flow}}(x) = \Delta_a q_a.$$

Note that this model is equivalent to (9.14) only if $\underline{\Delta}_a = 0$. However, this appears to be a moderate restriction in practice: it holds in all cases we have encountered. The complete MPEC type control valve model now reads:

$$0 = c_{a,\mathscr{E}}^{\text{mpec}}(x) = c_a^{\text{state}}(x),$$
$$0 \leq c_{a,\mathscr{I}}^{\text{mpec}}(x) = c_a^{\text{active-flow}}(x),$$
$$x_a = \begin{pmatrix} q_a \\ \Delta_a \end{pmatrix}.$$

9.1.7 ▪ Compressor groups

A compressor group $a = (u, v) \in A_{\text{cg}}$ usually has several compressor machines, powered by corresponding drives, to propel the gas by increasing its pressure (see Chapter 2). To serve a sufficiently broad range of operating conditions, i.e., flow-pressure combinations (q_a, p_u, p_v), every group has a suitable set $\mathscr{K}_a$ of technically possible *configurations*: serial combinations of parallel arrangements of compressor machines.

We introduce a triple $(q_{a,k}, p_{a,\text{in},k}, p_{a,\text{out},k})$ for every configuration $k \in \mathscr{K}_a$ and extend it to a variable vector $x_{a,k}$ to model the operation of configuration k with complete compressor machine and drive models. (In our smooth model formulation we will have $(q_{a,k}, p_{a,\text{in},k}) = (q_a, p_u)$, but $p_{a,\text{out},k} \neq p_v$ in general.) Now let $\mathscr{F}_{a,k}$ denote the set of *feasible* vectors $x_{a,k}$ in the sense that the gas pressure $p_{a,\text{in},k}$ can be increased to $p_{a,\text{out},k}$ at mass flow $q_{a,k}$ in configuration k. Moreover, choose a set of smooth constraints $c_{a,k,\mathscr{E}}^{\text{op-range}}, c_{a,k,\mathscr{I}}^{\text{op-range}}$ representing $\mathscr{F}_{a,k}$:

$$c_{a,k,\mathscr{E}}^{\text{op-range}}(x_{a,k}) = 0, \quad c_{a,k,\mathscr{I}}^{\text{op-range}}(x_{a,k}) \geq 0 \quad \Longleftrightarrow \quad x_{a,k} \in \mathscr{F}_{a,k}.$$

Details of these models are irrelevant here, but can be found in Schmidt, Steinbach, and Willert (2014) or Chapter 10.

Since only one configuration k can be active, we model the selection of a configuration with the special-ordered-set constraint

$$0 = c_a^{\text{sos}}(x) = \sum_{k \in \mathscr{K}_a} s_{a,k} - 1, \quad s_{a,k} \in \{0, 1\},$$

in combination with suitable big-M indicator constraints,

$$
\begin{aligned}
0 &\le c^{\text{ind-1}}_{a,k}(x) = M_{a,k,1}\left(1 - s_{a,k}\right) + c^{\text{op-range}}_{a,k,\mathscr{E}}(x_{a,k}),\\
0 &\le c^{\text{ind-2}}_{a,k}(x) = M_{a,k,2}\left(1 - s_{a,k}\right) - c^{\text{op-range}}_{a,k,\mathscr{E}}(x_{a,k}),\\
0 &\le c^{\text{ind-3}}_{a,k}(x) = M_{a,k,3}\left(1 - s_{a,k}\right) + c^{\text{op-range}}_{a,k,\mathscr{I}}(x_{a,k}).
\end{aligned}
$$

Here, $M_{a,k,i}, i = 1,2,3$, are vectors of big M's that are determined by estimations of the components of $c^{\text{op-range}}_{a,k,\mathscr{E}}$ and $c^{\text{op-range}}_{a,k,\mathscr{I}}$. Then the mixed-integer nonlinear model of the compressor group has variables

$$
x_a = \begin{pmatrix} (x_{a,k})_{k\in\mathscr{K}_a} \\ (s_{a,k})_{k\in\mathscr{K}_a} \end{pmatrix}
$$

and reads

$$
\begin{aligned}
0 &= c_{a,\mathscr{E}}(x) = c^{\text{sos}}_a(x),\\
0 &\le c_{a,\mathscr{I}}(x) = \left(c^{\text{ind-}i}_{a,k}(x)\right)^{i=1,2,3}_{k\in\mathscr{K}_a}.
\end{aligned}
$$

9.1.7.1 ▪ Compressor group model reformulation: Step 1—convex combination

Our key idea for finding a *feasible configuration* is based on a convex combination of all configurations with the following (fictitious) interpretation:

1. All configurations are simultaneously active in our model. As with the mixed-integer model, this allows conclusions on the feasibility of configurations.
2. All configurations have identical inflow gas pressures and serve the complete gas flow,

$$
\begin{aligned}
0 &= c^{\text{p-in-coupl}}_{a,k}(x) = p_u - p_{a,\text{in},k},\\
0 &= c^{\text{flow-distr}}_{a,k}(x) = q_a - q_{a,k}.
\end{aligned}
$$

3. The pressure increase $p_v - p_u$ of the entire group is a convex combination of pressure increases of the configurations with weights $\gamma_{a,k} \in [0,1]$:

$$
\begin{aligned}
0 &= c^{\text{press-inc}}_a(x) = p_v - p_u - \sum_{k\in\mathscr{K}_a} \gamma_{a,k}\left(p_{a,\text{out},k} - p_{a,\text{in},k}\right),\\
0 &= c^{\text{conv-combi}}_a(x) = \sum_{k\in\mathscr{K}_a} \gamma_{a,k} - 1.
\end{aligned}
$$

We remark that the constraints $c^{\text{op-range}}_{a,k,\mathscr{E}}$ and $c^{\text{op-range}}_{a,k,\mathscr{I}}$ ensure that $p_{a,\text{out},k} \ge p_{a,\text{in},k}$ holds. It might be possible in practice that more than one configuration can serve as a feasible active configuration for a given operating condition (q_a, p_u, p_v). For these cases, a selection method is described in Section 9.3.2. On the other hand, a given operating condition may be infeasible for some of the configurations. However, the corresponding weights can be set to zero so that the convex combination model is a feasible relaxation if (q_a, p_u, p_v) is feasible for at least one configuration.

9.1.7.2 ▪ Compressor group model reformulation: Step 2—relaxation

As the configurations of a group are designed to handle different operating conditions, their "overlap" is typically small: most of the concrete conditions (q_a, p_u, p_v) can only be handled by a few configurations. As a consequence, the above model will often be infeasible. The main reason for this is that every configuration has to compress the complete gas flow q_a, which is not always possible. Thus, we relax every set $\mathscr{F}_{a,k}$ to $\tilde{\mathscr{F}}_{a,k}$ with a standard slack formulation: we have $(x_{a,k}, \sigma_{a,k}) \in \tilde{\mathscr{F}}_{a,k}$ if there exist slack variables $\sigma_{a,k} \geq 0$ such that

$$\tilde{c}^{\text{op-range}}_{a,k,\mathscr{E}}(x_{a,k}, \sigma_{a,k}) = 0 \quad \text{and} \quad \tilde{c}^{\text{op-range}}_{a,k,\mathscr{I}}(x_{a,k}, \sigma_{a,k}) \geq 0.$$

Here the relaxed equality constraints are defined as

$$\tilde{c}^{\text{op-range}}_{a,k,\mathscr{E}}(x_{a,k}, \sigma_{a,k}) = c^{\text{op-range}}_{a,k,\mathscr{E}}(x_{a,k}) + \sigma^+_{a,k,\mathscr{E}} - \sigma^-_{a,k,\mathscr{E}},$$

the relaxed inequality constraints is given by

$$\tilde{c}^{\text{op-range}}_{a,k,\mathscr{I}}(x_{a,k}, \sigma_{a,k}) = c^{\text{op-range}}_{a,k,\mathscr{I}}(x_{a,k}) + \sigma^+_{a,k,\mathscr{I}},$$

and the complete slack vector is $\sigma_{a,k} = (\sigma^+_{a,k,\mathscr{E}}, \sigma^-_{a,k,\mathscr{E}}, \sigma^+_{a,k,\mathscr{I}})$. With $\sigma_a = (\sigma_{a,k})_{k \in \mathscr{K}_a}$, the relaxed convex combination model now reads

$$0 = c^{\text{rel-conv}}_{a,\mathscr{E}}(x, \sigma_a) = \begin{pmatrix} \left(c^{\text{flow-distr}}_{a,k}(x)\right)_{k \in \mathscr{K}_a} \\ c^{\text{press-inc}}_a(x) \\ c^{\text{conv-combi}}_a(x) \\ \left(c^{\text{p-in-coupl}}_{a,k}(x)\right)_{k \in \mathscr{K}_a} \\ \left(\tilde{c}^{\text{op-range}}_{a,k,\mathscr{E}}(x_{a,k}, \sigma_{a,k})\right)_{k \in \mathscr{K}_a} \end{pmatrix}, \tag{9.15a}$$

$$0 \leq c^{\text{rel-conv}}_{a,\mathscr{I}}(x, \sigma_a) = \left(\left(\tilde{c}^{\text{op-range}}_{a,k,\mathscr{I}}(x_{a,k}, \sigma_{a,k})\right)_{k \in \mathscr{K}_a} \right), \tag{9.15b}$$

$$x^{\text{rel-conv}}_a = \begin{pmatrix} q_a \\ (x_{a,k})_{k \in \mathscr{K}_a} \\ (\gamma_{a,k})_{k \in \mathscr{K}_a} \end{pmatrix}. \tag{9.15c}$$

We remark that the convex combination approach leads to the fact that (9.15) does not contain binary variables.

As usual, we try to enforce feasibility by minimizing the slacks $\sigma = (\sigma_a)_{a \in A_{\text{cg}}}$ in a suitable norm. This is also the objective of the entire smoothed MPEC:

$$f_{\text{sMPEC}}(\sigma) = \|\sigma\|.$$

9.1.8 ▪ Model summary

In the previous sections we have described components of gas transport networks, both as nonsmooth mixed-integer nonlinear models and, if necessary, as smooth MPEC reformulations. Now we collect the component models to obtain complete nMINLP and sMPEC formulations.

9.1.8.1 ▪ The complete nonsmooth mixed-integer nonlinear model

The complete feasibility problem in nMINLP form reads

$$\exists ?\, x : \quad c_{\mathscr{E},\text{nMINLP}}(x) = 0, \quad c_{\mathscr{I},\text{nMINLP}}(x) \geq 0,$$

where

$$c_{\mathscr{E},\text{nMINLP}}(x) = \begin{pmatrix} c_V(x) \\ c_{A_{\text{pi}}}(x) \\ c_{A_{\text{lin-rs}}}(x) \\ c_{A_{\text{nl-rs}}}(x) \\ c_{A_{\text{sc}}}(x) \\ c_{A_{\text{cg}},\mathscr{E}}(x) \end{pmatrix}, \quad c_{\mathscr{I},\text{nMINLP}}(x) = \begin{pmatrix} c_{A_{\text{va}}}(x) \\ c_{A_{\text{cv}}}(x) \\ c_{A_{\text{cg}},\mathscr{I}}(x) \end{pmatrix}$$

and

$$x = (x_V, x_{A_{\text{pi}}}, x_{A_{\text{lin-rs}}}, x_{A_{\text{nl-rs}}}, x_{A_{\text{sc}}}, x_{A_{\text{va}}}, x_{A_{\text{cv}}}, x_{A_{\text{cg}}})^T.$$

Here, nonsmooth aspects arise in all passive elements except for short cuts: $c_{A_{\text{pi}}}(x)$, $c_{A_{\text{lin-rs}}}(x)$, $c_{A_{\text{nl-rs}}}(x)$. Discrete decisions ("genuine" binary variables) arise in the active elements: $c_{A_{\text{cg}},\mathscr{E}}(x)$, $c_{A_{\text{cg}},\mathscr{I}}(x)$, $c_{A_{\text{va}}}(x)$, $c_{A_{\text{cv}}}(x)$. The node and short cut models $c_V(x)$, $c_{A_{\text{sc}}}(x)$ are smooth and will be kept in original form.

9.1.8.2 ▪ The complete smoothed MPEC model

Combining all smoothed and complementarity constrained component models, we obtain the following smooth MPEC model:

$$\min_{x,\sigma} \quad f_{\text{sMPEC}}(\sigma) \quad \text{s.t.} \quad c_{\mathscr{E},\text{sMPEC}}(x,\sigma) = 0, \quad c_{\mathscr{I},\text{sMPEC}}(x,\sigma) \geq 0, \tag{9.16}$$

where

$$c_{\mathscr{E},\text{sMPEC}}(x,\sigma) = \begin{pmatrix} c_V(x) \\ c^{\text{smooth}}_{A_{\text{pi}}}(x) \\ c^{\text{smooth}}_{A_{\text{lin-rs}}}(x) \\ c^{\text{smooth}}_{A_{\text{nl-rs}}}(x) \\ c_{A_{\text{sc}}}(x) \\ c^{\text{mpec}}_{A_{\text{va}}}(x) \\ c^{\text{mpec}}_{A_{\text{cv}},\mathscr{E}}(x) \\ c^{\text{rel-conv}}_{A_{\text{cg}},\mathscr{E}}(x,\sigma) \end{pmatrix}, \quad c_{\mathscr{I},\text{sMPEC}}(x,\sigma) = \begin{pmatrix} c^{\text{mpec}}_{A_{\text{cv}},\mathscr{I}}(x) \\ c^{\text{rel-conv}}_{A_{\text{cg}},\mathscr{I}}(x,\sigma) \end{pmatrix}, \tag{9.17}$$

and

$$x = \begin{pmatrix} x_V \\ x^{\text{smooth}}_{A_{\text{pi}}} \\ x_{A_{\text{lin-rs}}} \\ x^{\text{smooth}}_{A_{\text{nl-rs}}} \\ x_{A_{\text{sc}}} \\ x^{\text{mpec}}_{A_{\text{va}}} \\ x^{\text{mpec}}_{A_{\text{cv}}} \\ x^{\text{rel-conv}}_{A_{\text{cg}}} \end{pmatrix}, \quad \sigma = (\sigma_a)_{a \in A_{\text{cg}}}. \tag{9.18}$$

9.2 ▪ MPEC regularization

It is well known that MPEC models like (9.16) do not satisfy standard constraint qualifications (CQs), such as the *linear independence constraint qualification* (LICQ) or the *Mangasarian–Fromowitz constraint qualification* (MFCQ). As standard NLP solvers rely on such conditions, they cannot be applied directly to (9.16) without losing their theoretical convergence properties. In the literature one finds various regularization, smoothing, or penalization techniques to address this difficulty (see Scholtes (2001); DeMiguel et al. (2005); Hu and Ralph (2004)). Provided that the MPEC satisfies certain generalized CQs, they yield regular NLP formulations that depend on a (regularization, smoothing, or penalization) parameter $\tau > 0$. A sequence of parameters $\tau_\nu \to 0$ then yields a sequence of NLPs whose solutions converge to a solution of the given MPEC.

The standard penalization scheme turned out to be a very successful approach on our real-world instances. This scheme moves the complementarity constraints into the objective as a penalty term. More formally, given a general MPEC model

$$\begin{aligned} \min_{x} \quad & f(x) \\ \text{s.t.} \quad & c_{\mathcal{E}}(x) = 0, \quad c_{\mathcal{I}}(x) \geq 0, \\ & \phi_i(x)\psi_i(x) = 0, \quad i = 1, \ldots, k, \\ & \phi_i(x), \psi_i(x) \geq 0, \quad i = 1, \ldots, k, \end{aligned}$$

and a suitable penalty function π, the sequence of penalized NLPs is defined as

$$\begin{aligned} \min_{x} \quad & f(x) + \frac{1}{\tau_\nu} \sum_{i=1}^{k} \pi(\phi_i(x), \psi_i(x)) \\ \text{s.t.} \quad & c_{\mathcal{E}}(x) = 0, \quad c_{\mathcal{I}}(x) \geq 0, \\ & \phi_i(x), \psi_i(x) \geq 0, \quad i = 1, \ldots, k. \end{aligned}$$

A typical choice for the penalty function is $\pi(\phi_i(x), \psi_i(x)) = \phi_i(x)\psi_i(x)$.

For our purpose, solving an entire sequence of parameterized NLPs has two major drawbacks:

1. The sequence τ_ν is usually generated by a continuation technique and many parameterized NLPs may have to be solved until a given tolerance is reached. This contradicts the central goal of a primal heuristic, namely that it yields a feasible solution *quickly*.
2. The approach has the theoretical property that it only works if *every* parameterized NLP is solved successfully. However, our smoothed MPEC formulation is hard to solve because of potentially unstable smoothings and the large number of complementarity constraints. Thus, having to solve a large number of NLPs increases the risk of a failure.

To avoid these drawbacks, we solve only a *single* parameterized NLP where the parameter $\tau > 0$ is fixed at the value 10^{-6}, which proves to be a good value in our numerical experiments. The regular NLP reformulation of (9.16), rsMPEC, then reads

$$\begin{aligned} \min_{x,\sigma} \quad & f_{\text{rsMPEC}}(x, \sigma) := f_{\text{sMPEC}}(\sigma) + f_{\text{penalty}}(x) \\ \text{s.t.} \quad & c_{\mathcal{E},\text{rsMPEC}}(x, \sigma) = 0, \quad c_{\mathcal{I},\text{rsMPEC}}(x, \sigma) \geq 0, \end{aligned} \tag{9.19}$$

where $c_{\mathcal{E},\text{rsMPEC}}$ is constructed from $c_{\mathcal{E},\text{sMPEC}}$ by moving all complementarity constraints to the penalty term and keeping $c_{\mathcal{I},\text{rsMPEC}} = c_{\mathcal{I},\text{sMPEC}}$. The specific penalty term in our formulation is

$$f_{\text{penalty}}(x) = \frac{1}{\tau}\left(\sum_{a\in A_{\text{va}}} c_a^{\text{state}}(x)^2 + \sum_{a\in A_{\text{cv}}} c_a^{\text{state}}(x)^2\right),$$

where the squares are introduced to account for complementarity constraints that may become negative, such as $\tilde{p}_a q_a$ for valves ($\tilde{p}_a = p_u - p_v$) or control valves ($\tilde{p}_a = p_v - p_u + \Delta_a$).

9.3 ▪ Solution technique: A two-stage approach

In the previous sections, we have described how to transform the nonsmooth MINLP model into the regularized smooth MPEC model (9.19). This simplification comes at a price: the rsMPEC model, although in standard NLP form, is very hard to solve for most of our real-world instances. There are several reasons. First, the smoothing applied to nonsmooth constraints of pipes and resistors may lead to ill-conditioning and numerical instabilities. Second, rsMPEC involves a large number of penalized complementarity constraints in real-world instances, which may create additional numerical difficulties in the solution process. Finally, the convex combination model for compressor group configurations is highly nonlinear and nonconvex: it contains every compressor machine with full physical and technical details.

To overcome these difficulties we use a *two-stage approach* for solving (9.19). The goal of the first stage is to determine the major network flow situation including the discrete state of active elements and the directions of flow through resistors. In the second stage, these discrete decisions and flow directions are fixed, and the goal is to find feasible configurations for all active compressor groups.

9.3.1 ▪ Solving stage 1

In the first stage we try to determine a feasible flow situation in the network for the given nomination situation in terms of

1. the discrete states of valves, control valves, and compressor groups;
2. the directions of flow through resistors.

For this purpose we simplify the compressor group model substantially: rather than modeling configurations and operating ranges of compressor machines, we simply assume that every group can deliver a certain pressure increase $\Delta_a \in [0, \overline{\Delta}_a]$ that is independent of the flow. Here, $\overline{\Delta}_a$ is obtained by the preprocessing described in Section 5.4. The resulting MPEC formulation is similar to the MPEC model of control valves (Section 9.1.6):

$$0 = c_a^{\text{state}}(x) = \tilde{p}_a q_a, \quad 0 \le c_a^{\text{active-flow}}(x) = \Delta_a q_a,$$

with the pressure coupling variable

$$\tilde{p}_a := p_v - p_u - \Delta_a, \quad \Delta_a \in [0, \overline{\Delta}_a].$$

Thus, we have to replace $c_{a,\mathscr{E}}^{\text{rel-conv}}$, $c_{a,\mathscr{I}}^{\text{rel-conv}}$, $x_a^{\text{rel-conv}}$ in (9.15) by

$$\begin{aligned} 0 &= c_{a,\mathscr{E}}^{\text{simple}}(x) = c_a^{\text{state}}(x), \\ 0 &\le c_{a,\mathscr{I}}^{\text{simple}}(x) = c_a^{\text{active-flow}}(x), \end{aligned}$$

Table 9.1. *Fixing discrete states of valves.*

$\tilde{p}_a$	q_a	State	Binary variable
≈ 0	≈ 0	arbitrary	$s_a \in \{0,1\}$
≈ 0	$> \varepsilon_q$	open	$s_a = 1$
$> \varepsilon_p$	≈ 0	closed	$s_a = 0$
$> \varepsilon_p$	$> \varepsilon_q$	infeasible	—

Table 9.2. *Fixing discrete states of control valves and compressor groups.*

$\tilde{p}_a$	q_a	Δ_a	State	Binary variables	
≈ 0	≈ 0	≈ 0	arbitrary	$s_{a,1} \in \{0,1\}$	$s_{a,2} \in \{0,1\}$
≈ 0	≈ 0	$> \varepsilon_p$	closed	$s_{a,1} = 0$	$s_{a,2} = 0$
≈ 0	$> \varepsilon_q$	≈ 0	bypass or active	$s_{a,1} = 1$	$s_{a,2} \in \{0,1\}$
≈ 0	$> \varepsilon_q$	$> \varepsilon_p$	active	$s_{a,1} = 1$	$s_{a,2} = 1$
$> \varepsilon_p$	≈ 0	≈ 0	closed	$s_{a,1} = 0$	$s_{a,2} = 0$
$> \varepsilon_p$	≈ 0	$> \varepsilon_p$	closed	$s_{a,1} = 0$	$s_{a,2} = 0$
$> \varepsilon_p$	$> \varepsilon_q$	≈ 0	infeasible	—	
$> \varepsilon_p$	$> \varepsilon_q$	$> \varepsilon_p$	infeasible	—	

and

$$x_a^{\text{simple}} = \begin{pmatrix} q_a \\ \Delta_a \end{pmatrix}.$$

Our numerical experience shows that the first-stage solutions often have large flows in active elements that may lead to an infeasible second-stage model. Therefore we extend the first-stage objective to penalize flow in active elements,

$$f_{\text{rsMPEC-1}}(x) := f_{\text{penalty}}(x) + \sum_{a \in A_{\text{va}} \cup A_{\text{cv}} \cup A_{\text{cg}}} \omega_a q_a^2,$$

where $\omega_a \geq 0$ are instance-specific scaling factors. The objective term $f_{\text{sMPEC}}(x)$ of (9.19) is absent here, since we do not consider any configurations. Finally, the first-stage constraints and variables are obtained from (9.17) and (9.18) by replacing $c^{\text{rel-conv}}_{A_{\text{cg}},\mathscr{E}}, c^{\text{rel-conv}}_{A_{\text{cg}},\mathscr{I}}, x^{\text{rel-conv}}_{A_{\text{cg}}}$ with $c^{\text{simple}}_{A_{\text{cg}},\mathscr{E}}, c^{\text{simple}}_{A_{\text{cg}},\mathscr{I}}, x^{\text{simple}}_{A_{\text{cg}}}$.

9.3.2 ▪ Solving stage 2

The first-stage solution is used to fix discrete decisions and resistor flow directions in the second-stage model. Because of the penalization scheme used to regularize the complementarity constraints in the first-stage model (see Section 9.2), we cannot expect that the complementarity constraints hold exactly; this is only guaranteed in the limit $\tau \to 0$. Therefore, we choose pressure and flow tolerances $\varepsilon_p, \varepsilon_q > 0$ to decide whether $\tilde{p}_a$ or q_a are sufficiently small to be regarded as zero. This determines the discrete states of active elements according to Table 9.1 and Table 9.2. Finally, the resistor flow directions are fixed according to the sign of the flow variable.

The effects of fixing discrete states and resistor flow directions in Stage 2 are twofold. First, all nonsmooth aspects resulting from dependencies on flow directions are resolved.

Second, all discrete decisions of the underlying nonsmooth mixed-integer nonlinear program (MINLP) are fixed, except for the compressor group configurations. Thus, a smooth model can be formulated:

$$\begin{aligned}
\min_{x,\sigma} \quad & f_{\text{rsMPEC-2}}(\sigma) := f_{\text{sMPEC}}(\sigma) && && (9.20)\\
\text{s.t.} \quad & c_V(x) = 0, && c^{\text{smooth}}_{A_{\text{pi}}}(x) = 0,\\
& c_{A_{\text{sc}}}(x) = 0, && c^{\text{fix-flow}}_{A_{\text{lin-rs}}}(x) = 0,\\
& c^{\text{fix-flow}}_{A_{\text{nl-rs}}}(x) = 0, && c^{\text{fix-state}}_{A_{\text{va}}}(x) = 0,\\
& c^{\text{fix-state}}_{A_{\text{cv}}}(x) = 0, && c^{\text{rel-conv}}_{A_{\text{cg}},\mathscr{E}}(x,\sigma) = 0,\\
& c^{\text{rel-conv}}_{A_{\text{cg}},\mathscr{I}}(x,\sigma) \geq 0.
\end{aligned}$$

Here, the constraints selected by fixed discrete decisions read

$$0 = c^{\text{fix-state}}_a(x) = \begin{cases} p_u - p_v & \text{if } a \text{ is open},\\ q_a & \text{if } a \text{ is closed}, \end{cases}$$

for $a \in A_{\text{va}}$, and

$$0 = c^{\text{fix-state}}_a(x) = \begin{cases} p_u - p_v - \Delta_a & \text{if } a \text{ is active},\\ p_u - p_v & \text{if } a \text{ is in bypass mode},\\ q_a & \text{if } a \text{ is closed}, \end{cases}$$

for $a \in A_{\text{cv}}$. Finally, given resistor flows q^*_a of the first-stage solution, the discontinuous sgn term of the piecewise constant resistor model becomes constant,

$$0 = c^{\text{fix-flow}}_a(x) = p_u - p_v - \zeta_a \operatorname{sgn}(q^*_a), \quad a \in A_{\text{lin-rs}},$$

the nonsmooth term $q_a|q_a|$ in the piecewise quadratic model becomes $\operatorname{sgn}(q^*_a)q^2_a$ in $c^{\text{fix-flow}}_{A_{\text{nl-rs}}}$, and the unknown node index k in (9.8) is resolved as

$$k = \begin{cases} u & \text{if } q^*_a \geq 0,\\ v & \text{if } q^*_a < 0. \end{cases}$$

Selecting compressor group configurations After solving (9.20) it remains to decide on the configurations of active compressor groups. This is done in a heuristic way based on the convex coefficients $\gamma_{a,k}$ and the slack variables $\sigma_{a,k}$. To this end, let $\mathscr{K}_{a,\mathscr{F}}$ denote the set of configurations $k \in \mathscr{K}_a$ with vanishing slack variables,

$$\mathscr{K}_{a,\mathscr{F}} := \left\{ k \in \mathscr{K}_a : \left\| \sigma_{a,k} \right\| = 0 \right\}.$$

The decision is now made by the following case distinction:

1. If $|\mathscr{K}_{a,\mathscr{F}}| = 1$, choose the unique configuration $k \in \mathscr{K}_{a,\mathscr{F}}$.
2. If $|\mathscr{K}_{a,\mathscr{F}}| > 1$, choose $\operatorname{argmax}_{k \in \mathscr{K}_{a,\mathscr{F}}} \{\gamma_{a,k}\}$.
3. If $|\mathscr{K}_{a,\mathscr{F}}| = 0$, choose $\operatorname{argmin}_{k \in \mathscr{K}_a} \{\|\sigma_{a,k}\|\}$.

9.3.3 ▪ Conclusion

In this chapter, we presented reformulation techniques for the nonsmooth mixed-integer nonlinear problem of validation of nominations. These reformulation techniques cover the usage of complementarity constraints and a problem-specific convex combination approach for modeling the discrete parts of the model. In addition, all nonsmooth aspects are smoothed by standard or problem-specific approaches. The result is a smooth MPEC model, which is finally regularized by standard techniques from the literature in order to achieve an NLP that satisfies standard constraint qualifications. Thus, the final model can be solved by NLP solvers and the solutions can be used as approximative solution candidates for the NLP validation.

A drawback of this approach is that the reformulation of discrete aspects is not directly applicable to other discrete parts like subnetwork operation modes (see Section 2.4.3). As a consequence, this aspect is not regarded at all.

The main advantage of this approach is that all nonlinear aspects of the problem of validation of nominations can be included without significantly increasing the hardness of the problem. Thus, besides the complementarity constraints, the convex combination approach for compressor group configurations and all applied smoothings, the rsMPEC model contains the same model formulations as the ValNLP model.