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# Modelling compressor stations in gas networks

This report is a preliminary working paper presenting models for compressor stations that are used and developed in the Collaborative Research Centre TRR154 Mathematical Modelling, Simulation and Optimization using the Example of Gas Networks. The data files described in the appendix are available from the authors upon request. It is planned to provide them as part of the GasLib (http://gaslib.zib.de/).

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# Modelling compressor stations in gas networks

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#### Abstract

Gas networks are an important application area for optimization. When considering long-range transmission, compressor stations play a crucial role in these applications. This report collects and describes models for compressor stations. The emphasis is on recent work on simple yet accurate polyhedral models that may replace more simplified traditional models without increasing model complexity. The report also describes an extension of the compressor station data available in GasLib (http://gaslib.zib.de/) with the parameters of these models.

#### 1 Introduction

The long-range transmission of natural gas is driven by so-called compressor units, which are used to increase the gas pressure to ensure the flow of the gas through the network. Compressor units are organized in compressor stations that usually feature several compressor units which can be used in various configurations. This report summarizes models for compressor units and compressor stations that are intended to be used as part of a bigger optimization model.

The basic state variables for modeling an element of a gas network (e.g., a pipe, valve, or compressor unit) are the mass flow q along the network element and the inlet and outlet pressures  $p^{\rm in}$  and  $p^{\rm out}$ , respectively. Depending on the type of network element, the corresponding element model restricts values for these three state variables. The overall model for an entire gas network is then obtained by combining the element models via flow conservation and pressure coupling.

Detailed models of a compressor unit [4, 14] require additional variables and feature several nonlinear relations connecting all the variables. To model an entire compressor station, this model describing the technical behavior of a compressor unit is combined with a model describing the choice between several configurations for using the available compressor units, e.g., how many to use in parallel. Thus the detailed model for a compressor station is a nonlinear and nonconvex MINLP model. This level of detail is adequate for solving operational problems like minimizing the necessary compression power.

For many applications at the strategic and tactical level, e.g., expansion planning (see [1] and the references therein) and assessing the transmission capacity of the network [9], simpler models are sufficient. As in these applications one is often interested in globally optimal solutions, convex or even polyhedral models with few integer variables are of particular interest.

Recently, GasLib [13], a library with realistic gas network data, was created. GasLib is intended to be used as a common set of input data for comparing various approaches and techniques in gas network optimization. However, for compressor units the data comprises only the numerical parameters for the detailed model. Researchers that want to employ simplified models thus need to make up suitable numerical parameters for these models.

In this report, we describe several simplified models and how to derive their numerical parameters from the data for the detailed model. In particular, we focus on models in  $(q, p^{\rm in}, p^{\rm out})$ -space, i.e., models that avoid the additional variables for the technical details. The parameters of a simplified model are determined such that the approximation provided by it is as accurate as possible for this model type. This is useful in coarse-to-fine approaches (see e.g., [9]), where a coarse model is used to determine some high-level decisions that are later refined via a more detailed model. Moreover, we describe an extension of the original GasLib that makes these parameters available, thus extending the usefulness of the GasLib.

We consider only stationary models, i.e., models that are not time-dependent, in the isothermal case assuming a constant gas temperature T. To account for different gas temperatures in overall models taking into account changes in the gas temperature, we provide the numerical parameters for the models for various values of T.

The outline of the remaining report is as follows. Section 2 reviews the modeling concepts for compressor units and compressor stations introduced in [4]. In Section 3, we present several models for compressor units, starting with the detailed model from [4]. These models are then used in Sections 4 and 5 as building blocks for models of compressor stations. Table 1 provides an overview on the model described in this report. Appendix A describes the extension to the GasLib XML format for compressor units and stations that is used to provide the parameters for the simplified models.

# 2 Technical components and modeling elements of compressor stations

We use the following notions that have been proposed in [4].

Compressor machines are used to increase the pressure of the incoming gas to a higher outflow pressure. Thus, they satisfy the need to overcome pressure loss caused by friction in pipes and to transport gas over long distances. In present-day gas transport networks, one mainly finds turbo compressors and piston compressors in combination with one of four drive types: gas turbines, gas driven motors, electric motors and steam turbines. The combination of a compressor machine and a drive will be referred to as compressor unit.

Small groups of compressor machines and drives are often used together in such a way that the gas enters through a single pipe, is routed through some of the compressor machines, and leaves via a single pipe. To model this, we introduce the notion of *compressor groups*. These entities encapsulate a set of compressor machines (together with the corresponding drives) that can be operated in different predefined ways. Compressor groups are active elements, i.e., network operators can control their mode of operation. Technically possible

Model name	Equations	Model type	
Compressor unit level			
Physical model	(1b), (2), (3), (4), (13), (14)	nonconvex NLP	
	+ (6), (7), (8) (turbo) + (10), (12) (piston)		
Idealized model	(2), (16)	nonconvex NLP	
No-drive model	(17)	nonconvex NLP	
Polyhedral model $(Q, H_{ad})$	(3), (4), (18)	nonconvex NLP	
Polyhedral model $(q, p^{\text{in}}, p^{\text{out}})$	(19)	LP	
Box-constraint model	(21)	LP	
Configuration level			
Subnetwork model	(22) + machine model	(N)LP	
Polyhedral model $(q, p^{\text{in}}, p^{\text{out}})$	(19) on configuration level	$_{ m LP}$	
Box-constraint model	(21) on configuration level	LP	
Compressor group level			
Configuration choice model	(23) + configuration model	MI(NL)P	
Box-constraint model	(24)	LP	

Table 1: Overview of all models discussed in this report.

modes are active, closed, and bypass. If a compressor group is closed, it behaves like a closed valve. Thus, the gas flow is zero, and inflow and outflow gas states (i.e., gas pressure, temperature, and density) are decoupled. In bypass mode, the gas flows around the group and is therefore not affected by any part of the group. In active state, the compressor group can be operated in one of several different configurations, i.e., predefined arrangements of the single compressor machines. We define a configuration to be a serial combination of stages, where a stage in turn is a parallel combination of machines. Each machine must only occur at most once in every configuration. Figure 1 shows an example of a compressor group.

Frequently, collections of compressor machines are connected to more than two pipelines and may be used in various ways to route gas from some of those pipelines to other ones. Compressor groups are not sufficient to model such complex structures. Instead, for each *compressor station*, an explicit subnetwork that reflects all possible routes of gas through the compressor station is required. Similar to compressor groups, compressor stations internally allow for multiple paths that the flow of gas can actually take. The desired path is again selected by switching a cascade of individual valves, compressor groups, and (sometimes) control valves in the right way. An exemplary compressor station subnetwork with four different routings is shown in Figure 2.

In the following sections, we present models for compressor units, configurations and entire compressor groups.

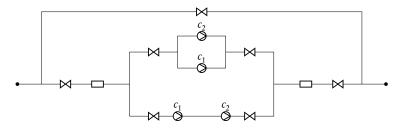
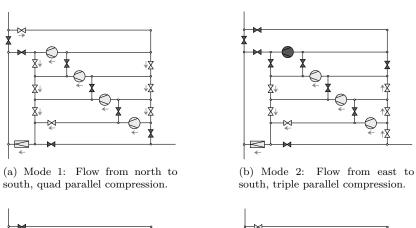
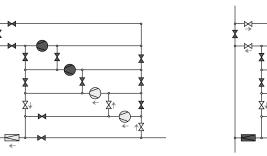


Figure 1: A compressor group with two compressors  $c_1, c_2$ , and two possible configurations. In the first configuration, the two compressors are connected in parallel. The second configuration consists of a serial connection of the same compressors. The bypass valve connected in parallel to the rest of the compressor group allows (uncompressed) flow in both directions.





(c) Mode 3: Flow from east to south, double serial compression.

(d) Mode 4: Flow from north to east with double and to south with single compression.

Figure 2: Four subnetwork operation modes representing different flows of gas through a large compressor station. Elements colored dark are "closed".

General gas-relate	d physical quantities		
Pressure	$\overline{p}$	[bar]	
Mass flow rate	q	[kg/s]	
Normal volumetric flow rate	$Q_0$	$[1000 m^3/h]$	
Temperature	T	[K]	
Density	ho	$[{\tt kg/m^3}]$	
Compressibility factor	z	[-]	
Pseudocritical temperature	$T_c$	[K]	
Pseudocritical pressure	$p_c$	[bar]	
Molar mass	$M_{ m mol}$	$[{\tt kg/kmol}]$	
Specific gas constant	$R_s$	$[\mathtt{kJ/(kg\cdot K)}]$	
Gas-related constants and conventions			
Standard temperature	$T_0 = 273.15$	[K]	
Standard pressure	$p_0 = 1.0$	[bar]	
Universal gas constant	R = 8.3144598	$[kJ/(kmol \cdot K)]$	
Quantities related to compressor units			
Specific change in adiabatic enthalpy	$H_{\mathrm{ad}}$	[kJ/kg]	
Volumetric flow rate	Q	$[m^3/s]$	
Power	$\stackrel{\cdot}{P}$	[kW]	
Specific energy consumption	b	[kW]	
Adiabatic efficiency	$\eta_{\mathrm{ad}} \in [0, 1]$	[-]	
Compressor speed	n	[rot./min]	
Isentropic exponent	$\kappa$	[-]	
Ambient temperature	$T_{ m amb}$	[°C]	
Absolute pressure increase	$\Delta$	[bar]	
Relative pressure increase	$\delta$	[-]	
Turbo compressor quantities			
Surgeline	quadratic polynomial		
Chokeline	quadratic polynomial		
Piston compr	essor quantities		
Shaft torque	M	[kNm]	
Operating volume	$V_o$	[m <sup>3</sup> /rot.]	

Table 2: General physical quantities and constants.

## 3 Models for compressor units

In this section we focus on models for compressor units. The description of the gas physics and the detailed technical model in Sections 3.1 and 3.2 are based closely on [4]. An overview on the physical quantities that are used in the models is given in Table 2. The constants provided in the formulas are based on the assumption that the values for all physical quantities are provided in the unit indicated in Table 2.

#### 3.1 Compressor-relevant gas physics

Before starting to describe the various models, we need to have a short look into the physics that play a role in the context of gas compression. A more detailed presentation can be found in e.g., [3, 4, 14].

The equation of state for ideal gases connects the state variables pressure p, density  $\rho$ , and temperature T and reads

$$p = \rho R_s T. \tag{1a}$$

The specific gas constant  $R_s$  can be computed from the universal gas constant R and the molar mass  $M_{\text{mol}}$  of the gas as  $R_s = RM_{\text{mol}}^{-1}$ . However, the properties of real gases differ from the above equation of state, which necessitates a correction by the so-called compressibility or real gas factor z = z(p, T). The modified equation of state is then

$$p = \rho R_s T z(p, T). \tag{1b}$$

For an ideal gas, z = 1.

The real gas factor depends on the chemical composition of the gas as well as on the pressure and the temperature. For low pressures and high temperatures, real gases behave almost ideally, whereas their properties differ significantly from those of ideal gases at higher pressures. There exist several approximations for the computation of the real gas factor, two of which we want to consider: First, the formula of the American Gas Association (AGA) is suitably precise up to a pressure of around 70 [bar]:

$$z(p,T) = 1 + 0.257 \frac{p}{p_c} - 0.533 \frac{p}{p_c} \frac{T_c}{T}.$$
 (2a)

Second, the formula of Papay is more accurate also for higher pressures:

$$z(p,T) = 1 - 3.52 \frac{p}{p_c} e^{-2.26 \frac{T}{T_c}} + 0.247 \left(\frac{p}{p_c}\right)^2 e^{-1.878 \frac{T}{T_c}}.$$
 (2b)

In both equations,  $p_c$  and  $T_c$  denote the pseudocritical pressure and temperature of the gas and depend on the composition of the gas. Figure 3 illustrates the two formulas for the compressibility factor for  $T=273.15\,[\mathrm{K}]$ .

Instead of regarding z as a variable, it can also be approximately seen as a constant parameter  $\overline{z}=z(\overline{p},\overline{T})$ . In the case of compressor machines, the relevant z-value is determined by the inlet pressure  $p^{\rm in}$ , such that the following is reasonable:

$$\overline{p} = \frac{1}{2}(p^{\text{in,min}} + p^{\text{in,max}}).$$

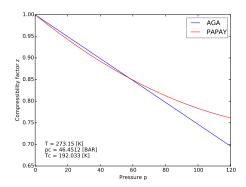


Figure 3: Compressibility factor computation.

#### 3.2 Physical models of compressor machines and drives

For a single compressor machine, the quantities that we are interested in comprise the inlet and outlet pressure  $p^{in}$  and  $p^{out}$  as well as the throughput of gas in terms of mass flow rate q. In each of the following models, these quantities will be subject to a set of constraints of varying complexity. The physical model that we will introduce first is the most detailed and realistic model used. It provides an accurate description of the physics of a compressor machine together with its compressor drive and is typically used in simulations and applications close to operations, e.g., in [2, 15, 12]. The physical model yields several nonlinearities that complicate the solving process of an optimization model. Therefore, it is also used as basis for the simplified models as described later in this chapter, with the goal of providing relaxations that reduce the complexity of the feasible operating range to a certain extent, respectively. As already mentioned, we distinguish between two types of compressor machines, turbo compressors and piston compressors, whose operational details are represented by different variables and restrictions. For more details and an extended discussion, we refer to [14].

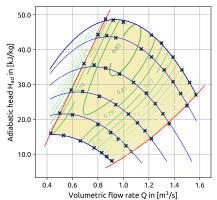
The feasible operating ranges of both turbo and piston compressors are given via so-called characteristic diagrams, that are, however, differently shaped. Examples of characteristic diagrams are shown in Figure 4. When the compressor machine is active, it must be operated at some point lying inside its characteristic diagram.

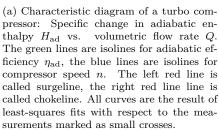
The two main quantities that restrict the capability of a compressor machine are the specific change in adiabatic enthalpy  $H_{\rm ad}$ , or adiabatic head, and the throughput in terms of volumetric flow Q, given by:

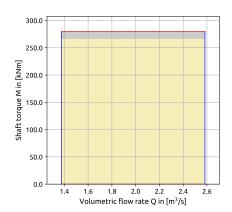
$$H_{\rm ad} = R_s T z^{\rm in} \frac{\kappa}{\kappa - 1} \left[ \left( \frac{p^{\rm out}}{p^{\rm in}} \right)^{\frac{\kappa - 1}{\kappa}} - 1 \right], \tag{3}$$

$$Q = \frac{q}{\rho^{\text{in}}}.\tag{4}$$

The adiabatic head takes a positive value if the outlet pressure  $p^{\text{out}}$  is higher than the inlet pressure  $p^{\text{in}}$ , which is always the case for an active turbo compressor machine. If the two were equal as for a switched-off machine,  $H_{\text{ad}}$  would be







(b) Characteristic diagram of a piston compressor: Shaft torque M vs. volumetric flow rate Q. The blue lines represent the minimum and maximum speed, the upper red line the maximal compression ratio in terms of shaft torque M.

Figure 4: Characteristic diagrams of compressor machines.

zero. The mass flow q through an active machine is always positive, which directly yields positivity for the volumetric flow Q, whereas the flow through an inactive machine is zero. Via the thermodynamical standard equation for real gases (1b), now respecting the units in Table 2, the gas density at the inlet  $\rho^{\rm in}$  is given as

$$\rho^{\rm in} = 100 \frac{p^{\rm in}}{z^{\rm in} R_s T},\tag{5}$$

with  $z^{\rm in}=z(p^{\rm in},T)$ . The factor 100 comes from unit conversion:  $1[{\tt bar}]=100\,[{\tt kJ/m^3}]$ . Assuming a constant compressibility factor, which is a common simplification in this context, leads to a linear proportional relation between pressure and density.

#### 3.2.1 Turbo compressors

The boundaries of the characteristic diagram of a turbo compressor are determined by applying least-squares quadratic fits to measurement points. The same is true for the isolines of speed and adiabatic efficiency. As a result, we have (bi)quadratic polynomials for which we use the following notation:

$$\chi(x,y;A) = \begin{pmatrix} 1 \\ x \\ x^2 \end{pmatrix}^T \begin{pmatrix} a_{00} & a_{01} & a_{02} \\ a_{10} & a_{11} & a_{12} \\ a_{20} & a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} 1 \\ y \\ y^2 \end{pmatrix},$$
$$\psi(x;a) = a_0 + a_1 x + a_2 x^2.$$

We assume that all coefficients are available for our models.

The left and the right boundaries of the characteristic diagram are called *surgeline* and *chokeline*, respectively, whereas the lower and upper boundaries result from operating the machine at minimum and maximum speed. The corresponding inequalities are given as follows:

$$H_{\rm ad} \le \psi(Q; a^{\rm surge}),$$
 (6a)

$$H_{\rm ad} \ge \psi(Q; a^{\rm choke}),$$
 (6b)

$$H_{\rm ad} \le \psi(Q; a^{\rm speedMin}),$$
 (6c)

$$H_{\rm ad} \ge \psi(Q; a^{\rm speedMax}).$$
 (6d)

The compressor speed n of an active turbo compressor is only implicitly given via a biquadratic equation relating speed, flow and adiabatic head:

$$H_{\rm ad} = \chi(Q, n; A^{\rm speed}).$$
 (7)

There are, however, explicit bounds on the compressor speed:  $n \in [n^{\min}, n^{\max}]$ . The adiabatic efficiency  $\eta_{\rm ad}$  always takes a value in [0, 1] and can be explicitly obtained from

$$\eta_{\rm ad} = \chi(Q, n; A^{\rm eff}). \tag{8}$$

Notice that the two equations (7) and (8) are only valid within the boundaries of the characteristic diagram. Hence, n and  $\eta_{\rm ad}$  are left undefined if the machine is switched off and must be manually set to some meaningful value (e.g. zero).

#### 3.2.2 Piston compressors

In contrast to turbo compressors, piston compressors have a constant adiabatic efficiency  $\overline{\eta}_{\rm ad}$ .

They are characterized by their operating volume  $V_o$ , i.e., the volume of gas that can be compressed in every rotation of the piston. The volumetric flow Q and the compressor speed n are related via this operating volume (with  $1 [\min] = 60 [s]$ ):

$$Q = \frac{nV_o}{60}. (9)$$

Same as for turbo machines, n is explicitly bounded by  $n^{\min}$  and  $n^{\max}$ . With the above equation, these bounds can be used to compute bounds on Q:

$$Q \in [Q^{\min}, Q^{\max}] \tag{10}$$

Moreover, piston compressors can be characterised by their shaft torque M:

$$M = \frac{V_o H_{\rm ad} \rho^{\rm in}}{2\pi \bar{\eta}_{\rm ad}}.$$
 (11)

Since  $H_{\rm ad}=0$  for an inactive compressor (with all quantities in the denominator being strictly positive), a shaft torque value of zero is implied in that case. However, the characteristic diagram of piston compressors technically also allows

for zero shaft torque and thus zero compression if the machine is active. From a modelling point of view, this might not be a desirable behavior since, within a compressor group, it is already covered by the bypass mode. As a remedy, one could impose a small minimum shaft torque value  $M^{\min} > 0$  that every active machine must at least achieve.

For some piston compressors, the maximum torque value  $M^{\rm max}$  is known and can then be directly used, while in other cases only a maximum relative or absolute compression ratio  $\delta^{\rm max}$  or  $\Delta^{\rm max}$  is given. Respectively, one of the following three restrictions is incorporated:

$$M \le M^{\text{max}},\tag{12a}$$

$$p^{\text{out}} \le p^{\text{in}} \delta^{\text{max}},$$
 (12b)

$$p^{\text{out}} \le p^{\text{in}} + \Delta^{\text{max}}.$$
 (12c)

#### 3.2.3 Compressor drives

Each compressor machine is powered by a compressor drive. Again, there exist several types: Electric motors, gas driven motors, gas turbines and steam turbines. However, we will use a mathematical model that is general enough to incorporate all of them. The power that is required for the compression process is given by

$$P = \frac{\rho^{\rm in}QH_{\rm ad}}{\eta_{\rm ad}} = \frac{qH_{\rm ad}}{\eta_{\rm ad}}.$$
 (13)

In the case of an inactive turbo compressor, where  $\eta_{\rm ad}$  is undefined, the value of P also remains undefined and must be explicitly set to zero.

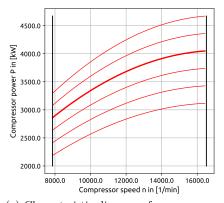
The maximal power that a drive can deliver to a compressor machine may depend on the compressor speed and the ambient temperature and is again given as a (bi)quadratic polynomial. Furthermore, every compressor drive has an individual energy consumption rate b that is, in general, a quadratic function of the power produced. See Figure 5 for an example.

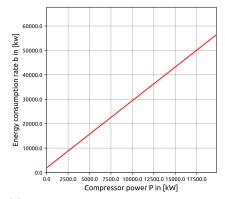
$$P \le P^{\text{max}} = \begin{cases} \chi(n, T_{\text{amb}}; A^{\text{power}}), \\ \psi(n; a^{\text{power}}) \end{cases}$$
 (14)

$$b = \psi(P, a^{\text{energy}}). \tag{15}$$

#### 3.3 Simplified models

Depending on the application and the overall optimization model, using the detailed physical model from Section 3.2 as a building block may be too complex. Also, detailed compressor unit data such as characteristic diagrams may not be available, e.g., in network expansion applications where the compressor units do not exist yet and the goal is to determine some general design parameters like the required maximum compression power. For these reason, simplified compressor models have been developed.





(a) Characteristic diagram of a compressor drive: Compressor speed n vs. power P. The red lines show the maximal power that the drive can deliver at different ambient temperatures  $T_{\rm amb}$ . Lower temperatures allow for higher power.

(b) Energy consumption of a compressor drive: Power P vs. energy consumption rate b. In general, the function can be quadratic, here it is only linear.

Figure 5: Characteristic diagrams of compressor drives.

These simplified compressor models are usually "less nonlinear" than the detailed physical model. Of particular interest are models that are linear or mixed-integer linear, as these can be integrated in common MILP optimization models for gas networks without leaving the realm of MILP models. The simplifications are achieved by neglecting nonlinear constraints and some of the "internal" state variables like the adiabatic efficiency  $\eta_{\rm ad}$  and the compressor speed n.

#### 3.3.1 Idealized models

As mentioned in [14], earlier work on gas network optimization often consider idealized models of compressor machines and drives, see e.g., [11, 10]. These models incorporate the basic physical relations shared by turbo and piston compressors: specific change in adiabatic enthalpy (3) and power consumption (13). However, they assume a constant adiabatic efficiency  $\bar{\eta}_{\rm ad}$  and they replace characteristic diagrams and drive properties with simple bounds on the compressor power,  $P^{\rm min}$  and  $P^{\rm max}$ . Analogously, bounds on q and  $H_{\rm ad}$  may be used as well. These bounds are either given explicitly or may be derived from the detailed physical model if the idealized model is to be used as an approximation for it,

see Section 3.3.4. Altogether, the model reads as follows:

$$H_{\rm ad} = R_s T z^{\rm in} \frac{\kappa}{\kappa - 1} \left[ \left( \frac{p^{\rm out}}{p^{\rm in}} \right)^{\frac{\kappa - 1}{\kappa}} - 1 \right], \tag{16a}$$

$$qH_{\rm ad} \le \overline{\eta}_{\rm ad} P^{\rm max},$$
 (16b)

$$qH_{\rm ad} \ge \overline{\eta}_{\rm ad} P^{\rm min},$$
 (16c)

$$q \in [q^{\min}, q^{\max}], \tag{16d}$$

$$H_{\text{ad}} \in [H_{\text{ad}}^{\text{min}}, H_{\text{ad}}^{\text{max}}].$$
 (16e)

This model is often used in applications where the goal is to minimize the compressor power for handling a given gas demand. In fact, assuming a constant adiabatic efficiency  $\bar{\eta}_{\rm ad}$  and a constant energy consumption rate  $\bar{b}$  (cf. (15)), the term  $qH_{\rm ad}$  provides the exact value for the compressor power in the detailed physical model.

Another very simple relaxation of the physical model results from assuming no restrictions on the power that can be delivered. That is, it is only ensured that  $(Q, H_{ad})$  or (Q, M) lie within the characteristic diagram of a turbo or piston compressor, whereas all constraints related to the power (i.e., (8) and (13)) as well as to the compressor drive ((14), (15)) are omitted:

$$\rho^{\rm in} = \frac{p^{\rm in}}{R_{\circ}Tz^{\rm in}} \tag{17a}$$

$$z^{\rm in} = z(p^{\rm in}, T)$$
 according to (2)

$$H_{\rm ad} = R_s T z^{\rm in} \frac{\kappa}{\kappa - 1} \left[ \left( \frac{p^{\rm out}}{p^{\rm in}} \right)^{\frac{\kappa - 1}{\kappa}} - 1 \right], \tag{17c}$$

$$Q = \frac{q}{\rho^{\text{in}}} \tag{17d}$$

$$M = \frac{V_o H_{\rm ad} \rho^{\rm in}}{2\pi \overline{\eta}_{\rm ad}} \quad \text{(only for piston compressors)}$$
 (17e)

+ feasibility for compressor machine: 
$$(6)$$
 or  $(10)$ , $(12)$   $(17f)$ 

#### 3.3.2 Polyhedral model in $(Q, H_{ad})$ -space

Going one step further than the no-drive model in terms of removing nonlinearities, we might want to consider a linearized and convexified version of the characteristic diagram boundary. This only applies to turbo compressors since the characteristic diagrams of piston compressors already have these properties. Typically, only one or two of the four boundary lines of a turbo compressor characteristic diagram are slightly concave, such that the convexification error is relatively small. The linearization error that is made depends on the amount of support points used. Having computed such an outer approximation as a set of polytope facets  $\mathcal{F}$ , we can add linear facet inequalities

$$a_f Q + b_f H_{\text{ad}} + c_f \le 0 \qquad \forall f \in \mathcal{F}$$
 (18)

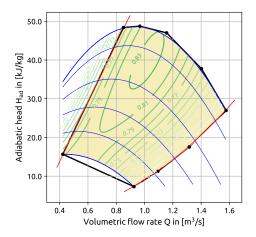


Figure 6: Linear outer approximation of a characteristic diagram.

instead of the characteristic diagram boundary inequalities (6a)-(6d). However, the entire model remains nonlinear due to the nonlinear relations of Q and  $H_{\rm ad}$  to our main problem variables q,  $p^{\rm in}$  and  $p^{\rm out}$ . An example of a linearized characteristic diagram is shown in Figure 6.

#### 3.3.3 Polyhedral model in $(q, p^{in}, p^{out})$ -space

As we have seen, the capabilities of a compressor machine are determined by its characteristic diagram. However, incorporating the respective characteristic diagram variables,  $(Q, H_{ad})$  for turbo compressors and (Q, M) for piston machines, into a model yields difficulties due to their nonlinear relation to the main problem variables  $(q, p^{in}, p^{out})$ . Hence, the idea of the polyhedral model is to find linear models in the  $(q, p^{in}, p^{out})$ -space, given by a set  $\mathcal{F}$  of polyhedral facets

$$a_f q + b_f p^{\text{in}} + c_f p^{\text{out}} + d_f \le 0 \qquad \forall f \in \mathcal{F}$$
 (19)

based on transformations of the original characteristic diagrams.

**Turbo compressors** In this paragraph, we follow closely the steps presented in [6] in order to derive a polyhedral description of the feasible region of turbo compressors in  $(q, p^{\text{in}}, p^{\text{out}})$ . As for turbo compressors, recall that we have the following mapping, given by equations (3) and (4):

$$\begin{pmatrix} Q \\ H_{\mathrm{ad}} \end{pmatrix} = f(q, p^{\mathrm{in}}, p^{\mathrm{out}}) = \begin{pmatrix} \frac{100qR_sTz^{\mathrm{in}}}{p^{\mathrm{in}}} \\ R_sTz^{\mathrm{in}} \frac{\kappa}{\kappa - 1} \left[ \left( \frac{p^{\mathrm{out}}}{p^{\mathrm{in}}} \right)^{\frac{\kappa - 1}{\kappa}} - 1 \right] \end{pmatrix} \in \mathbb{R}^2.$$

Conversely, a point  $(Q, H_{ad})$  can be transformed into a (curved) ray in the  $(q, p^{in}, p^{out})$ -space. There is one degree of freedom in this transformation, which we represent by the variable p. The curvature comes from the evaluation of the compressibility factor z = z(p, T) according to the formulas of PAPAY or

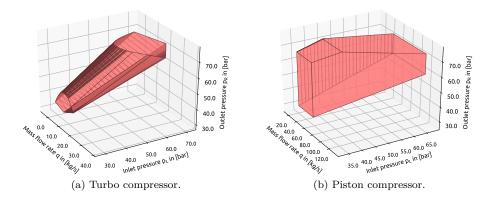


Figure 7: The operating range polytopes of the two different compressor machine types in  $(q, p^{\text{in}}, p^{\text{out}})$ .

AGA. If we assume z to be constant, then all rays would be linear in p for fixed  $(Q, H_{ad})$ :

$$\begin{pmatrix} q \\ p^{\text{in}} \\ p^{\text{out}} \end{pmatrix} = g(Q, H_{\text{ad}}; p) = \begin{pmatrix} \frac{Qp}{100R_sTz} \\ p \\ \left(\frac{H_{\text{ad}}}{R_sTz\frac{\kappa}{\kappa-1}} + 1\right)^{\frac{\kappa}{\kappa-1}} p \end{pmatrix} \in \mathbb{R}^3 \quad \text{for } p \ge 0.$$

Whereas in [6] a constant z-factor is assumed, the impact of working with the PAPAY or AGA formula has been studied in [5].

In practice, we start the construction with a set of characteristic diagram points  $\{(Q^{(k)}, H_{\rm ad}^{(k)})\}_{k=1}^n$ , e.g., the measurements or some random sample. Applying the above mapping yields a set of rays in  $(q, p^{\rm in}, p^{\rm out})$ . On all of these rays, we compute discrete points using sample values for the free variable p. For each of the generated points  $\{(q^{(k)}, p^{{\rm in}(k)}, p^{{\rm out}(k)})\}_{k=1}^m$ , we then compute the value of the required compressor power P according to (13) and compare it to the power bound (14). Points that are infeasible w.r.t. the power bound are discarded. This step is an addition to the procedure described in [6] and is also analysed in [5]. Let C denote the convex hull of all the remaining power-feasible points. In order to a obtain a linear approximation to the feasible operating range of the compressor unit in  $(q, p^{\rm in}, p^{\rm out})$ , we finally intersect C with half-spaces corresponding to the technical limitations of the compressor machine:

$$p^{\text{in}} \ge p^{\text{in,min}},$$
  
 $p^{\text{out}} \le p^{\text{out,max}},$   
 $q \ge q^{\text{min}},$   
 $q < q^{\text{max}}.$ 

The constraint  $p^{\text{out}} \geq p^{\text{in}}$  should be implicitly fulfilled through nonnegative  $H_{\text{ad}}$ -values in the characteristic diagram, but can of course be explicitly added.

**Piston compressors** For piston compressors, the dependencies between the problem variables  $(q, p^{\text{in}}, p^{\text{out}})$  and the compressor variables (Q, M) are simpler.

Assuming that we are only given the pressure bounds  $p^{\text{in,min}}$  and  $p^{\text{out,max}}$ , we can immediately use these for the remaining bounds:

$$p^{\text{in,max}} := p^{\text{out,max}},$$
  
 $p^{\text{out,min}} := p^{\text{in,min}}.$ 

As long as  $p^{\mathrm{in,min}} \leq p^{\mathrm{out,max}}$ , these bounds are valid and also tight, since piston compressors technically allow for an arbitrarily small pressure increase.

The mass flow bounds  $q^{\min}$  and  $q^{\max}$  can be directly derived from the bounds on the volumetric flow Q in the characteristic diagram. From the equations (5) and (4), we obtain  $q = \frac{100Qp^{\text{in}}}{RTz^{\text{in}}}$ . This becomes minimal for  $Q = Q^{\min}$  and  $p^{\text{in}} = p^{\text{in,min}}$ , and maximal for  $Q = Q^{\max}$  and  $p^{\text{in}} = p^{\text{in,max}}$  (since the compressibility factor  $z^{\text{in}}$  is monotonously decreasing in  $p^{\text{in}}$ ), such that we get

$$q \geq q^{\min} = \frac{100Q^{\min}p^{\text{in,min}}}{RTz^{\text{in}}},$$

$$q \leq q^{\rm max} = \frac{100Q^{\rm max}p^{\rm in,max}}{RTz^{\rm in}}.$$

If upper bounds on the absolute or relative pressure increase  $\Delta$  or  $\delta$  are available, they are added as

$$\begin{split} p^{\text{out}} &\leq p^{\text{in}} + \Delta^{\text{max}}, \\ p^{\text{out}} &\leq p^{\text{in}} \delta^{\text{max}}. \end{split}$$

If a maximal shaft torque value  $M^{\max}$  is given, we can use equation (11) to derive a maximal compression ratio  $\delta^{\max}$  as follows:

$$\delta = \frac{p^{\text{out}}}{p^{\text{in}}} = \left(\frac{M^{\text{max}} 2\pi \eta_{\text{ad}}}{V_o \frac{\kappa}{\kappa - 1} p^{\text{in}}} + 1\right)^{\frac{\kappa}{\kappa - 1}} \to \text{max} \qquad \Leftrightarrow \qquad p^{\text{in}} = p^{\text{in,min}}. \tag{20}$$

Figure 7 illustrates the resulting operating ranges in  $(q, p^{\text{in}}, p^{\text{out}})$ -space of both a turbo and a piston compressor.

#### **3.3.4** Box-constraint model in $(q, p^{in}, p^{out})$ -space

For solving optimization problems on large networks that involve compressor stations, the physical compressor machine model is far too complex. However, it is solvable when a machine is considered individually. Hence, we can precompute bounds on our variables of interest  $(p, p^{\rm in}, p^{\rm out})$  as well as on the absolute and relative pressure increase,  $\Delta$  and  $\delta$ , via the physical model NLP and then build a simpler compressor model upon these. The same idea has already been applied to the compressor power P in the idealized model.

The model then reads as follows:

$$q \in [q^{\min}, q^{\max}], \tag{21a}$$

$$p^{\text{in}} \in [p^{\text{in,min}}, p^{\text{in,max}}],$$
 (21b)

$$p^{\text{out}} \in [p^{\text{out,min}}, p^{\text{out,max}}],$$
 (21c)

$$p^{\rm out} - p^{\rm in} \in [\Delta^{\rm min}, \Delta^{\rm max}], \tag{21d}$$

$$\frac{p^{\text{out}}}{p^{\text{in}}} \in [\delta^{\text{min}}, \delta^{\text{max}}]. \tag{21e}$$

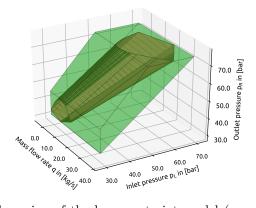


Figure 8: Feasible region of the box-constraint model (green) compared with the feasible region of the polyhedral model in  $(q, p^{\text{in}}, p^{\text{out}})$  as in Figure 7a.

Notice that the results depend on the assumed ambient and gas temperature. Figure 8 shows a typical feasible region of the box-constraint model.

#### 4 Configuration models

As described in the beginning, compressor machines are operated in one of several technically possible configurations within a compressor group. By convention and thereby covering all practically relevant cases, we assume a configuration to be a sequence of parallel compressor machine arrangements. The variables  $p^{in}$  and  $p^{out}$  shall now refer to the inlet and outlet pressure of the configuration, and q denotes its throughput in terms of mass flow, such that our target space of interest remains  $(q, p^{in}, p^{out})$ .

#### 4.1 Subnetwork model

Most obviously, configurations can be modelled as a simple subnetwork consisting of serially combined stages of parallel machines with pressure coupling and flow conservation constraints. Formally, for a configuration, let  $\mathcal{T} = \{t_1 \dots t_k\}$ be an ordered set of k serial stages. Every stage  $t \in \mathcal{T}$  comprises a set  $\mathcal{M}_t = \{m_1^{(t)} \dots m_{l_k}^{(t)}\}$  of compressor machines that are operated in parallel. For each stage  $t \in \mathcal{T}$ , we introduce in- and out-pressure variables  $p_t^{\text{in}}$  and  $p_t^{\text{out}}$ , respectively. Moreover, for every compressor machine  $m \in \mathcal{M}_t$ ,  $\forall t \in \mathcal{T}$ , we introduce a (nonnegative) mass flow variable  $q_{t,m}$ . With this, the subnetwork model can be stated as follows:

$$q = \sum_{m \in \mathcal{M}_t} q_{t,m} \qquad \forall t \in \mathcal{T}$$

$$p^{\text{in}} = p_{t_1}^{\text{in}}$$

$$(22a)$$

$$p^{\rm in} = p_{t_1}^{\rm in} \tag{22b}$$

$$p_i^{\text{out}} = p_{i+1}^{\text{in}} \qquad \forall i = 1 \dots k - 1 \tag{22c}$$

$$p_i^{\text{out}} = p_{i+1}^{\text{in}} \qquad \forall i = 1 \dots k-1$$

$$p^{\text{out}} = p_{t_k}^{\text{out}}$$

$$(22d)$$

$$(q_{t,m}, p_t^{\text{in}}, p_t^{\text{out}}) \in \mathcal{P}_{t,m}$$
  $\forall t \in \mathcal{T} \, \forall m \in \mathcal{M}_t,$  (22e)

where  $\mathcal{P}_{t,m}$  denotes the set of feasible working points of some arbitrary compressor unit model from Section 3.

# 4.2 Polyhedral model in $(q, p^{in}, p^{out})$ -space

Following the steps described in [6] and similar to the polyhedral model for compressor machines, the goal is again to find a linear model for the overall capabilities of a configuration in the space of  $(q, p^{\text{in}}, p^{\text{out}})$ .

Let us start with finding the representation of the operating range for a single stage, i.e., the parallel combination of compressor machines. For simplicity of the notation, we assume that there are only two parallel machines  $M_1$  and  $M_2$ , but the extension to the general case is straight-forward. Let

$$P_{M_1} := \{ (q_1, p_1^{\text{in}}, p_1^{\text{out}}) \},$$
  

$$P_{M_2} := \{ (q_2, p_2^{\text{in}}, p_2^{\text{out}}) \}$$

denote the feasible operating ranges of  $M_1$  and  $M_2$  as determined by the polyhedral model of a single compressor machine. Then, the feasible region of the parallel combination  $M_1 \parallel M_2$  can be described as

$$P_{M_1||M_2} := \{(q, p^{\text{in}}, p^{\text{out}})\}$$

with

$$q = q_1 + q_2$$

$$p^{\text{in}} = p_1^{\text{in}} = p_2^{\text{in}} \qquad \text{for} \qquad (q_1, p_1^{\text{in}}, p_1^{\text{out}}) \in P_{M_1},$$

$$p^{\text{out}} = p_1^{\text{out}} = p_2^{\text{out}} \qquad (q_2, p_2^{\text{in}}, p_2^{\text{out}}) \in P_{M_2}.$$

In words, the mass flows simply add up while the in- and out-pressure must be equal for both machines.

Having computed the overall operating range of each stage, we need to proceed with finding the operating range of their serial combination. Again, we restrict ourselves to the case of two serial stages  $S_1$  and  $S_2$  whose operating ranges are given by all points in

$$P_{S_1} := \{ (q_1, p_1^{\text{in}}, p_1^{\text{out}}) \},$$
  

$$P_{S_2} := \{ (q_2, p_2^{\text{in}}, p_2^{\text{out}}) \}.$$

In the serial combination  $S_1 \to S_2$ , the mass flow through both machines must be equal and the outlet pressure of stage  $S_1$  must match the inlet pressure of stage  $S_2$ . The feasible region of  $S_1 \to S_2$  is then given as

$$P_{S_1 \to S_2} := \{(q, p^{\text{in}}, p^{\text{out}})\}$$

with

$$q = q_1 = q_2$$
 
$$p^{\text{in}} = p_1^{\text{in}} \qquad (q_1, p_1^{\text{in}}, p_1^{\text{out}}) \in P_{S_1},$$
 
$$p^{\text{out}} = p_2^{\text{out}} \qquad (q_2, p_2^{\text{in}}, p_2^{\text{out}}) \in P_{S_2}.$$
 
$$p_1^{\text{out}} = p_2^{\text{in}}$$

Obviously, while parallel combinations of machines are always symmetric, the order of serially combined stages matters. In general, the resulting operating range of serial combination  $S_1 \to S_2$  is different to the one of  $S_2 \to S_1$ .

### 4.3 Box-constraint model in $(q, p^{in}, p^{out})$ -space

The idea of the box-constraint model as presented in the previous Section 3.2 for individual compressor machines can also be generalized to configurations. As a preprocessing step, we now compute bounds on several quantities by solving NLPs based on the physical compressor model in combination with the above-mentioned subnetwork model for the configuration. In this case, we focus on bounds within the  $(q, p^{\rm in}, p^{\rm out})$ -space. Bounds on the adiabatic head  $H_{\rm ad}$  and the volumetric flow Q could of course also be included, but are not as meaningful for an entire configuration as they were for a single machine. With  $\Delta$  and  $\delta$  referring to the absolute and relative pressure increase, respectively, the model can be written (similar to the box-constraint machine model) as

$$\begin{split} q &\in [q^{\min}, q^{\max}], \\ p^{\text{in}} &\in [p^{\text{in,min}}, p^{\text{in,max}}], \\ p^{\text{out}} &\in [p^{\text{out,min}}, p^{\text{out,max}}], \\ p^{\text{out}} &- p^{\text{in}} \in [\Delta^{\min}, \Delta^{\max}], \\ \frac{p^{\text{out}}}{p^{\text{in}}} &\in [\delta^{\min}, \delta^{\max}]. \end{split}$$

The box-constraint model for configurations is superior to the one for individual machines, since it provides a tighter relaxation and necessitates fewer variables. For example, let us consider two machines  $M_1$  and  $M_2$  that are serially combined and let  $\delta_1^{\max}$  and  $\delta_2^{\max}$  denote their respective maximal compression ratios as computed by the box-constraint machine model. Then, the subnetwork model for the configuration would assume the maximal overall compression ratio to be  $\delta^{\max} = \delta_1^{\max} \cdot \delta_2^{\max}$ . However,  $\delta_1^{\max}$  and  $\delta_2^{\max}$  may have been achieved by  $M_1$  and  $M_2$  at very different rates of mass flow. This is automatically taken into account by the box-constraint configuration model, which yields  $\delta^{\max} \leq \delta_1^{\max} \cdot \delta_2^{\max}$ .

# 5 Compressor group models

In the previous section, we have described several models for configurations of multiple compressor machines. Now, we want to widen our view and find models for an entire compressor group that consists of several configurations and whose capabilities shall, again, be characterized by the tuple of variables  $(q, p^{\text{in}}, p^{\text{out}})$ . As we have mentioned before, compressor groups can be in different states: closed or open, and, if open, active or bypass. At this point, we will focus on active compressor groups.

#### 5.1 Configuration choice model

In an active compressor group, exactly one of the configurations must be active. Therefore, let  $P_i$ , i=1...n, denote the operating range of configuration i as obtained by any of the configuration models, with n being the number of possible configurations. Furthermore, we introduce a binary variable  $s_i$  for

every configuration i with

 $s_i = 1$ , if configuration i is active,  $s_i = 0$ , otherwise.

With this, we can formulate a first and very flexible model (with respect to the configuration and machine models that are used):

$$s_i = 1 \quad \Rightarrow \quad (q, p^{\text{in}}, p^{\text{out}}) \in P_i,$$
 (23a)

$$\sum_{i=1}^{n} s_i = 1, \tag{23b}$$

$$s_i \in [0, 1], \quad i = 1 \dots n.$$
 (23c)

#### 5.2 Box-constraint model

Starting with the parameter bounds computed for the box-constraint configuration model, we immediately develop a variant of that model for a compressor group. For any parameter  $\xi \in \{q, p^{\text{in}}, p^{\text{out}}, \Delta, \delta\}$ , let  $\xi_i^{\text{min}}$  and  $\xi_i^{\text{max}}$  denote the bounds of this parameter computed for configuration  $i, i = 1 \dots n$ . Then, we can directly determine overall parameter bounds for the compressor group as

$$\begin{split} \xi^{\min} &:= \min_{i=1...n} \{\xi_i^{\min}\}, \\ \xi^{\max} &:= \max_{i=1...n} \{\xi_i^{\max}\}, \end{split}$$

and use these in a similar way as in the box-constraint model for compressor machines or configurations.

However, we can easily do better: For every configuration i=1...n, the intersection of the half-spaces given by the parameter bound inequalities yields a polyhedral feasible set  $P_i$  of points in the same space of  $(q, p^{\text{in}}, p^{\text{out}})$ . We can then use the convex hull of the union of all these polyhedra to impose:

$$(q, p^{\mathrm{in}}, p^{\mathrm{out}}) \in \operatorname{conv} \bigcup_{i=1}^{n} P_i.$$

For this, we do not explicitly need to compute  $\bigcup_{i=1}^n P_i$ , but can use a convex combination of the vertices  $v(P_i)$  of all  $P_i$ ,  $i=1\ldots n$ :

$$(q, p^{\text{in}}, p^{\text{out}}) = \sum_{v \in \bigcup v(P_i)} \lambda_v v \quad \text{with} \quad \sum_{v \in \bigcup v(P_i)} \lambda_v = 1, \ \lambda_v \ge 0.$$
 (24)

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#### References

- [1] Conrado Borraz-Sánchez, Russell Bent, Scott Backhaus, Hassan Hijazi, and Pascal Van Hentenryck. Convex relaxations for gas expansion planning. *INFORMS J. Comp.*, 28(4):645–656, 2016.
- [2] R.G. Carter. Compressor station optimization: Computational accuracy and speed. Technical Report PSIG 9605, Pipeline Simulation Interest Group, 1996.
- [3] Günter Cerbe. Grundlagen der Gastechnik: Gasbeschaffung Gasverteilung Gasverwendung. Technik. Hanser Verlag, Leipzig, Germany, 2008.
- [4] Armin Fügenschuh, Björn Geißler, Ralf Gollmer, Antonio Morsi, Marc E. Pfetsch, Jessica Rövekamp, Martin Schmidt, Klaus Spreckelsen, and Marc C. Steinbach. Physical and technical fundamentals of gas networks. In Koch et al. [8].
- [5] B. Hiller, R. Saitenmacher, and T. Walther. Polyhedral 3d models for compressors in gas networks. ZIB-Report 17-66, Zuse Institute Berlin, 2017.
- [6] Jesco Humpola, Armin Fügenschuh, Benjamin Hiller, Thorsten Koch, Thomas Lehmann, Ralf Lenz, Robert Schwarz, and Jonas Schweiger. The specialized MINLP approach. In Koch et al. [8].
- [7] Jesco Humpola, Imke Joormann, Nikolaos Kanelakis, Djamal Oucherif, Marc E. Pfetsch, Lars Schewe, Martin Schmidt, Robert Schwarz, and Mathias Sirvent. GasLib – A Library of Gas Network Instances. Report, Optimization Online, 2017. http://www.optimization-online.org/DB\_ HTML/2015/11/5216.html.
- [8] Thorsten Koch, Benjamin Hiller, Marc Pfetsch, and Lars Schewe, editors. Evaluating Gas Network Capacities. MOS-SIAM Series on Optimization. SIAM, 2015.
- [9] Thorsten Koch, Benjamin Hiller, Marc E. Pfetsch, and Lars Schewe. Evaluating Gas Network Capacities. MOS-SIAM Series on Optimization. SIAM, 2015.
- [10] D. Mahlke, A. Martin, and S. Moritz. A mixed integer approach for timedependent gas network optimization. Opt. Meth. and Soft., 25(4):625–644, 2010.
- [11] A. Martin, M. Möller, and S. Moritz. Mixed integer models for the stationary case of gas network optimization. *Math. Programming*, 105(2):563–582, 2006.
- [12] Daniel Rose, Martin Schmidt, Marc C. Steinbach, and Bernhard M. Willert. Computational optimization of gas compressor stations: MINLP models versus continuous reformulations. *Math. Methods Oper. Res.*, 83(3):409–444, 2016.

- [13] Martin Schmidt, Denis Aßmann, Robert Burlacu, Jesco Humpola, Imkes Joormann, Nikolaos Kanelakis, Thorsten Koch, Djamal Oucherif, Marc E. Pfetsch, Lars Schewe, Robert Schwarz, and Mathias Sirvent. GasLib – A Library of Gas Network Instances. Preprint, TRR 154, 2017. https://opus4.kobv.de/opus4-trr154/frontdoor/index/index/docId/168.
- [14] Martin Schmidt, Marc C. Steinbach, and Bernhard M. Willert. High detail stationary optimization models for gas networks. *Optimization and Engineering*, 16(1):131–164, 2015.
- [15] Martin Schmidt, Marc C. Steinbach, and Bernhard M. Willert. The precise NLP model. In Koch et al. [8].

# A Extended XML format for compressor models

All of the models presented in this report can be set up using the publicly available data from the GasLib [7]. This library of gas network data contains several network instances together with detailed specifications of compressor units and different flow-pressure-scenarios in standard XML format. The compressor groups as arcs in the gas network are specified in the .net-file, whereas all specific data related to the compressor units and configurations within a compressor group is given in the corresponding .cs-file.

We have extended the format of the Gaslib .cs-file in order to accomodate the data of some of the simplified models. The numerical values for the compressor models do depend to some extent on the composition of the gas. To obtain specific values, we used the parameters of pure methane  $(CH_4)$ :

```
\begin{split} M_{\rm mol} &= 16.043\,[{\rm kg/kmol}] \\ R_s &= 0.5182705\,[{\rm kJ/(kg\cdot K)}] \\ p_c &= 45.922\,[{\rm bar}] \\ T_c &= 190.564\,[{\rm K}] \\ \kappa &= 1.304 \end{split}
```

The quantity  $\kappa$ , the so-called isentropic exponent, actually depends both on the gas composition as well as on the gas temperature. We use  $\kappa = 1.304$  independently of the chosen gas temperature value. In order to account for the dependency of the compressor model parameters on the gas temperature, we decided to include data for various gas temperatures, namely  $\{0, 15, 30, 45\}$  [°C].

To provide the model parameters, we extended the existing XML format for compressor data by a new tag <boxModelBounds> which is added both on the level of compressor units and on the level of configurations. The parameters of the gas composition that have been assumed are documented in the parameters> subtag.

The values for the computed bounds follow in a tag of the form <gasTemperature unit="K" value="273.15">. The values of the bounds themselves are specified, for each of the physical quantities, together with their respective unit, as for example

```
<massFlowMin unit="kg_per_s" value="22.5201"/>
<massFlowMax unit="kg_per_s" value="131.4391"/>.
```

Moreover, we incorporated facet inequalities of the polytope approximations of the characteristic diagrams in  $(Q, H_{\rm ad})$  as well as the operating range in  $(q, p^{\rm in}, p^{\rm out})$ . These are supposed to be used in addition to the bounds. They are given specified and listed within an <code><additionalFacets>-tag</code>, where the attribute <code><space="ppq"> refers</code> to the operating range in  $(q, p^{\rm in}, p^{\rm out})$  and <code><space="QHad"> the characteristic diagram in  $(Q, H_{\rm ad})$ . A comprehensive example of the added XML format is given in Figure 9.</code>

```
<boxModelBounds>
 <parameters>
   <compressibilityFactorFormula value="papay"/>
   <pseudocriticalPressure unit="bar" value="45.922"/>
   <molarMass unit="kg_per_kmol" value="16.043"/>
   <ambientTemperature unit="Celsius" value="10.0"/>
   <isentropicExponent unit="1" value="1.304"/>
   <pseudocriticalTemperature unit="K" value="190.564"/>
   <specificGasConstant unit="kJ_per_kg_per_K" value="0.518260911301"/>
 </parameters>
 <gasTemperature unit="K" value="273.15">
   <massFlowMin unit="kg_per_s" value="22.5201"/>
   <massFlowMax unit="kg_per_s" value="131.4391"/>
   cpressureInMin unit="bar" value="31.0132"/>
   cpressureOutMin unit="bar" value="32.6953"/>
   oressureOutMax unit="bar" value="71.0132"/>
   sureIncAbsMin unit="bar" value="1.682"/>
   cpressureIncRelMin unit="1" value="1.0542"/>
   <adiabaticHeadMin unit="kJ_per_kg" value="6.8858"/>
   <adiabaticHeadMax unit="kJ_per_kg" value="48.9912"/>
   <volumetricFlowMin unit="m_cube_per_s" value="0.9409"/>
   <volumetricFlowMax unit="m_cube_per_s" value="3.3796"/>
   <normVolumetricFlowMin unit="1000m_cube_per_hour" value="114.4246"/>
   <normVolumetricFlowMax unit="1000m_cube_per_hour" value="667.8426"/>
   <powerMin unit="kW" value="339.6328"/>
   -
<powerMax unit="kW" value="3383.575"/>
   <additionalFacets space="ppq">
     <variables>
       <variable coeff="a" name="massFlow" unit="kg_per_s"/>
       <variable coeff="b" name="pressureIn" unit="bar"/>
<variable coeff="c" name="pressureOut" unit="bar"/>
     <facet a="0.0755" b="0.6691" c="-0.7393" rel="le" rhs="-0.3221"/>
     facet a="-0.0450" b="0.7560" c="-0.6530" rel="le" rhs="0.2734"/>
   </additionalFacets>
   <additionalFacets space="QHad">
     <variables>
       <variable coeff="a" name="volumetricFlow" unit="m_cube_per_s"/>
       <variable coeff="b" name="adiabaticHead" unit="kJ_per_kg"/>
     </variables>
     <facet a="-0.9885" b="-0.1514" rel="le" rhs="-2.7158"/>
     <facet a="-0.9999" b="0.0165" rel="le" rhs="-0.7246"/>
     <facet a="-0.9998" b="0.0215" rel="le" rhs="-0.5494"/>
   </additionalFacets>
 </gasTemperature>
 <gasTemperature unit="K" value="288.15">
 </gasTemperature>
</boxModelBounds>
```

Figure 9: Example excerpt from the extended XML data for the compressor models.