

Analytical and Algebraic Approaches to Gas Transportation with Uncertain Loads

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Abstract

Since the deregulation of the natural gas industry new challenges and tasks concerning the transportation of gas arose. This brought into life a whole new research field dealing with models and problem formulations satisfying the new needs of the natural gas industry. Being a difficult task even before the deregulation, the task of gas transportation became even more complex because uncertainty plays a more important role now. In this context, the computation of the probability of feasibility of exit load vectors in passive steady-state gas networks, which is addressed in this thesis, is a task of high importance.

Passive steady-state gas networks can be modeled via an algebraic system taking into account Kirchhoff's first and second law. A characterization for feasibility of load vectors that reduces the number of variables is utilized to compute the probability of exit load vectors to be feasible with spheric-radial decomposition. For solving systems of multivariate polynomial equations Gröbner basis techniques are used. With this method networks with up to three fundamental cycles that are not edge-disjoint can be analyzed. Two methods to reduce the number of polynomial systems to be solved are presented. First, some rules for possible flow directions along the pipes are given and an upper bound for the number of possible flow directions is deduced. Second, a method for finding redundant pressure bounds is given.

Parametric optimization problems arising in model predictive control are of high interest. Hence, it is an important task to identify an explicit representation of the set of feasible load vectors. In a mathematical context this means that systems of parametric quadratic multivariate polynomials have to be solved. This problem is tackled by extending Gröbner bases to comprehensive Gröbner systems, which yield parametric Gröbner bases.

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Symbols

General Notation

\mathbb{N}	the set of natural numbers
$\mathbb{Z}, \mathbb{Z}_{\geq 0}$	the set of (nonnegative) integers
$\mathbb{Z}^n, \mathbb{Z}_{\geq 0}^n$	the set of (nonnegative) integer column vectors of dimension n
\mathbb{Q}	the set of rational numbers
\mathbb{R}	the set of real numbers
\mathbb{C}	the set of complex numbers
\emptyset	the empty set
\mathbb{S}^{n-1}	$(n - 1)$ -dimensional unit sphere in \mathbb{R}^n
$ S $	the cardinality of a set S
$ s $	the absolute value of a number s
$ v $	componentwise absolute value of a vector v , $(v)_i = v_i $
$v v $	componentwise, $(v v)_i = v_i v_i $
v^2	componentwise square of a vector v , $(v^2)_i = (v_i)^2$
e_i	the i -th unit vector
I_n	the identity matrix of dimension n
$A_{i,\bullet}$	the i -th row of a matrix A
$A_{\bullet,j}$	the j -th column of a matrix A
A_M	the matrix consisting of the columns of A that are indexed by the elements of M
v_M	the vector consisting of the components of v that are indexed by the elements of M
$\text{diag}(v)$	the diagonal matrix whose diagonal is v
\subseteq	subset relation where equality can occur
\subset	strict subset relation where equality must not occur
\mathbb{P}	probability
ξ	a random vector
μ	the mean value of a distribution
R	the correlation matrix of a distribution
Σ	the covariance matrix of a distribution
$\mathcal{N}(\mu, \Sigma)$	(multivariate) Gaussian distribution with mean value μ and covariance matrix Σ

\mathcal{S}	a set of samples
v	a sample
\mathcal{H}_a	the hyperplane generated by the arc a

Algebra

k	a field
\bar{k}	algebraic closure of a field k
k^n, \bar{k}^n	n -dimensional affine space over k and \bar{k} , respectively
$k[x_1, \dots, x_n]$	the set of all polynomials in x_1, \dots, x_n with coefficients in k , the polynomial ring
$k[u_1, \dots, u_m][x_1, \dots, x_n]$	the set of all polynomials in x_1, \dots, x_n with coefficients in $k[u_1, \dots, u_m]$
f, g, h, p, q, r	polynomials in $k[x_1, \dots, x_n]$
x_1, \dots, x_n, x, y, z	indeterminates
$\text{totaldeg}(x^\alpha)$	the total degree of a monomial x^α
$\text{deg } f$	the total degree of a polynomial f
\mathcal{I}, \mathcal{J}	ideals
$\langle f_1, \dots, f_s \rangle$	the ideal generated by polynomials f_1, \dots, f_s
\mathcal{V}, \mathcal{W}	affine varieties
$\mathbf{V}(f_1, \dots, f_s)$	the variety defined by polynomials f_1, \dots, f_s
$\mathbf{V}(\mathcal{I})$	the variety defined by the polynomials in \mathcal{I}
$\mathbf{I}(\mathcal{V})$	the set of all polynomials that vanish on \mathcal{V} , the ideal of \mathcal{V}
$\sqrt{\mathcal{I}}$	the radical of an ideal \mathcal{I}
\succeq	monomial ordering on the monomials in $k[x_1, \dots, x_n]$
$\text{multideg}(f)$	the multidegree of a polynomial f
$\text{lc}(f)$	the leading coefficient of a polynomial f
$\text{lm}(f)$	the leading monomial of a polynomial f
$\text{lt}(f)$	the leading term of a polynomial f
$\text{lt}(\mathcal{I})$	the set of leading terms of the elements of \mathcal{I}
$\text{lcm}(f, g)$	the least common multiple of monomials f and g
$r_F(f)$	the remainder on division of a polynomial f by the set of polynomials F
\mathcal{G}	a Gröbner basis of an ideal in $k[x_1, \dots, x_n]$
$S(f, g)$	the S -polynomial of polynomials f and g
\mathcal{I}_l	the l -th elimination ideal of an ideal \mathcal{I}
\mathcal{G}_l	a Gröbner basis of the l -th elimination ideal
\equiv	congruence relation
$[f]$	the equivalence class of a polynomial f for congruency modulo an ideal
$k[x_1, \dots, x_n]/\mathcal{I}$	the quotient of the polynomial ring $k[x_1, \dots, x_n]$ modulo an ideal \mathcal{I}
$\dim_K R$	the Krull dimension of a ring R

σ	specialization of $k[u_1, \dots, u_m]$ or $k[u_1, \dots, u_m][x_1, \dots, x_n]$
σ_a	specialization induced by $a \in \bar{k}^m$
$\tilde{\mathcal{G}}$	a comprehensive Gröbner system of a set of polynomials in $k[u_1, \dots, u_m][x_1, \dots, x_n]$

Graph Theory

G	a graph or digraph
\vec{G}	an orientation of a graph G
$V, V(G)$	the set of all nodes of a (directed) graph
$A, A(G)$	the set of all edges (arcs) of a (directed) graph
u, v, w	nodes
r	the root node of a spanning tree
a, b, c	edges (arcs)
$N_G(u)$	the set of all neighbors of a node u in the (directed) graph G
$\deg(u)$	the degree of a node u
$\deg^{\text{in}}(u)$	the in-degree of a node u
$\deg^{\text{out}}(u)$	the out-degree of a node u
$\text{head}(a)$	the head of an arc a in a directed graph
$\text{tail}(a)$	the tail of an arc a in a directed graph
\mathcal{T}	a tree
$\overline{\mathcal{T}}$	the cotree of a spanning tree \mathcal{T} in a (directed) graph
$u\mathcal{T}v$	the unique path from node u to node v in a spanning tree \mathcal{T}
$D_{\mathcal{T}}(u)$	the set of all descendants of a node u w.r.t. a search-tree \mathcal{T}
$p(u)$	the predecessor of a node u w.r.t. a search-tree
C^+	the set of all cycles in a graph
$C = C_{\mathcal{T}}$	the set of all fundamental cycles in a (directed) graph w.r.t. a spanning tree \mathcal{T}
C_a	the set of all fundamental cycles in a (directed) graph that contain the edge (arc) a
\mathcal{C}	a cycle
\mathcal{C}_a	the fundamental cycle containing the non-tree edge (arc) a
$a_{\mathcal{C}}$	the non-tree edge (arc) in $A(\overline{\mathcal{T}})$ that generates the fundamental cycle $\mathcal{C} \in C_{\mathcal{T}}$
$A_{C'}$	the set of all edges (arcs) $a \in A$ that are edges (arcs) of the fundamental cycles in C' but not of those in $C \setminus C'$
\mathcal{A}^+	the incidence matrix of a (directed) graph
\mathcal{A}	the reduced incidence matrix of a (directed) graph

\mathcal{A}_B	the matrix consisting of the columns of \mathcal{A} that correspond to the edges (arcs) of a spanning tree of the (directed) graph
\mathcal{A}_N	the matrix consisting of the columns of \mathcal{A} that correspond to the edges (arcs) of the cotree of a spanning tree of the (directed) graph
$\mathcal{B} = \mathcal{B}_T$	the fundamental cycle matrix of a (directed) graph w.r.t. the spanning tree \mathcal{T}
\mathcal{B}_B	the matrix consisting of the rows of \mathcal{B} that correspond to the edges (arcs) of a spanning tree of the (directed) graph
\mathcal{B}_N	the matrix consisting of the rows of \mathcal{B} that correspond to the edges (arcs) of the cotree of a spanning tree of the (directed) graph
$\mathcal{P} = \mathcal{P}_T$	the path matrix of a digraph w.r.t. a spanning tree \mathcal{T}

Gas Network Modeling

V^+	the set of junctions/nodes
V_+	the set of entry nodes
V_-	the set of exit nodes
V_0	the set of innodes
$r \in V_+$	root of the spanning tree, reference node of the network
V	the set of nodes without the reference node
A	the set of pipes
$Q_0, Q_{0,a}$	volumetric flow rate under normal conditions in $\text{m}^3 \text{h}^{-1}$ (along pipe a)
Q_0	vector in $\mathbb{R}^{ A }$ of volumetric flow rates
p, p_u	pressure of the gas in Pa (at junction u)
p^+, p	vectors in $\mathbb{R}^{ V^+ }$ and $\mathbb{R}^{ V }$, respectively, of pressures
$\underline{p}_u, \bar{p}_u$	lower respectively upper pressure bound of the gas at junctions u in Pa
$\underline{p}^+, \underline{p}, \bar{p}^+, \bar{p}$	vectors in $\mathbb{R}^{ V^+ }$ and $\mathbb{R}^{ V }$, respectively, of pressure bounds
$q^{\text{nom}}, q_u^{\text{nom}}$	load in $\text{m}^3 \text{h}^{-1}$ (at junction u)
$q^{\text{nom}+}, q^{\text{nom}}$	vectors in $\mathbb{R}^{ V^+ }$ and $\mathbb{R}^{ V }$, respectively, of loads
M	the set of feasible load vectors
M_-	the set of feasible exit load vectors (if the network contains exactly one entry node)
$M_-(v)$	the set of $r \in \mathbb{R}_{\geq 0}$ s.t. $rLv + \mu$ is a feasible exit load
$S \subseteq \{-1, 1\}^{ A }$	the set of all feasible resolvings of the absolute values

P_s	the set of all indices such that the corresponding pressure bound inequality is nonredundant, $s \in S$
ϕ	pressure drop coefficient of the gas in a specific pipe
$\Phi = \text{diag}(\phi_{a_1}, \dots, \phi_{a_m})$	diagonal matrix of pressure drop coefficients of arcs a_i , $i = 1, \dots, m$
ρ	density of the gas in kg m^{-3}
ρ_0	density of the gas under normal conditions in kg m^{-3}
v	velocity of the gas in m s^{-1}
m	molar mass of the gas in kg mol^{-1}
η	dynamic viscosity of the gas in Pa s
T	temperature of the gas in K
T_c	(pseudo-)critical temperature of the gas in K
p_c	(pseudo-)critical pressure of the gas in Pa
p_m	mean pressure of the gas in Pa
q	massflow in kg s^{-1}
R_s	specific gas constant of the gas in $\text{J kg}^{-1} \text{K}^{-1}$
z	compressibility factor of the gas
$z_m = z(p_m, T)$	mean compressibility factor of the gas
$z_0 = z(p_0, T_0)$	compressibility factor under normal conditions of the gas
$\lambda = \lambda(Q_0)$	friction factor of the gas in a specific pipe
$\text{Re} = \text{Re}(Q_0)$	Reynolds number of the gas in a specific pipe
A	cross-sectional area of pipe in m^2
D	diameter of a pipe in m
k	integral roughness of the inner pipe wall in m
s	slope of a pipe, in $[-1, 1]$
L	length of a pipe in m
x	location in a pipe, in $[0, L]$
t	time in s

Constants

$g = 9.80665 \text{ m s}^{-2}$	gravitational acceleration
$T_0 = 273.15 \text{ K}$	norm temperature
$p_0 = 101325 \text{ Pa}$	norm pressure
$R = 8.31441 \text{ J mol}^{-1} \text{ K}^{-1}$	universal gas constant

*“We all use math every day;
to predict weather, to tell time, to handle money.
Math is more than formulas or equations;
it’s logic, it’s rationality,
it’s using your mind to solve the biggest mysteries we know.”*

– NUMB3RS

Chapter 1

Introduction

Since the deregulation of the natural gas industry in Europe in the 2000s, and before that in the USA in the 1990s, new challenges and tasks concerning the transportation of gas arose. This brought into life a whole new research field dealing with models and problem formulations satisfying the new needs of the natural gas industry. Being a difficult task even before the deregulation, the task of gas transportation became even more complex because uncertainty plays a more important role now. Previously, gas companies have been gas traders and network operators at the same time, but since the deregulation of the natural gas industry these companies had to split up and now they either trade gas or operate the pipeline systems. Gas transport customers first have to book with a transmission system operator (TSO) rights to inject or withdraw gas up to a certain amount at corresponding injection and withdrawal points of the pipeline system. Then, one day before the booked gas transport is planned to take place, the transport customers have to nominate to what extend and where they plan to exercise their rights. This leads to the fact that the TSO has to ensure that all nominations that are theoretically possible within the bookings are physically and technically feasible. If he can not accomplish such a nomination, he has to pay penalty fees to the customers whose contracts could not been satisfied.

The natural gas flow can be modeled independent of time (steady-state models) or dependent of time (transient models). In transient models the relations between different quantities such as pressure and flow are described through partial differential equations. This makes it difficult to integrate transient models in optimization problems. However, in steady-state models the partial differential equations reduce to algebraic nonlinear equations. These equations model Kirchhoff's first and second law, conservation of mass and loop rule, cf. [65, 66]. The loop rule states that the pressure drop within a cycle sums up to zero. It turns out that the existence of cycles in a pipeline system complicates the solution of natural gas flow problems. Ríos-Mercado and Borraz-Sánchez [99] write:

“While the size of a gas pipeline system definitely plays an important role when solving natural gas network flow problems, it is the network topology that really defines the complexity of the model, e.g., cyclic

networks are extremely more difficult to solve than its (gun-barrel and tree-shaped) network counterparts.”

Ríos-Mercado et al. [99] and Iliadis et al. [63] give overviews of the optimization problems arising in the natural gas industry. One optimization problem is the line-packing problem. By injecting more gas into the system than is withdrawn, which is possible since gas is compressible, the pipeline system can be used as a short-term storage. When the stored gas is needed, there can be withdrawn more gas than is injected. These two procedures are called line-packing and line-drafting. The task here is to find a sufficient level of line-pack during a given planning horizon. The model of de Nevers and Day in [36] identifies the limits of line-packing and line-drafting for a single pipeline segment in an unsteady-state pipeline system. In [28] and [106] the line-packing problem is examined under consideration of uncertain future load.

Another interesting problem is the pooling problem occurring in gas and oil pipeline systems. If the system contains gas or oil of different sources, and with that of different quality, it is an important question how to operate the system and how to mix the different gas resp. oil streams in order to fulfill given customer requirements. The modeling involves bilinear and convex quadratic programming constraints called quality constraints. The pooling problem is investigated in, e.g., [4, 14, 44, 61], and in a stochastic setting in [8, 13]. Moreover, in [5] it is proven that the pooling problem is NP-hard.

In addition to that, an aspect of essential importance is the (optimal) design of a network. This aspect is split into two issues. The first one is to create a whole new network, the second one is to add new elements such as pipes or compressors to an existing network. The optimal design of pipeline systems is addressed in, e.g., [7, 11, 30, 42, 76, 78, 80].

The most effort has been put into the minimum fuel cost problem that addresses the optimal operation of the compressors of the network. The reason for this is that the operating cost of compressor stations ranges between 25% and 50% of the company’s total operating cost, cf. [54]. Steady-state models are the ones in [18, 27, 72, 73] where dynamic programming is utilized to solve the problem. While [72, 73] consider linear and tree-structured pipeline systems, [18, 27] investigate pipeline systems with at least one cycle containing compressors. Moreover, [43, 91] use a gradient search and [81, 93] apply mixed integer nonlinear programming tools. Transient models are examined in [29, 40, 46, 79, 90, 97, 98]. While these models focus on the continuous modeling of compressors, the transient models of [26, 59, 75] include discrete decisions concerning, e.g., (control) valves.

All those optimization problems have in common that one of their constraints is feasibility of the gas flow. When uncertainty comes into play two different approaches are possible. If the uncertainty is stochastic, i.e., its distribution is known, this constraint is replaced by a probabilistic constraint stating that the probability that the gas flow is feasible is greater than a given benchmark. For a

survey on probabilistic constraints see, e.g., [95] and [94]. If the uncertain variable is fully unknown, robust optimization is utilized to solve the problem, c.f. [15]. Both approaches are outlined with application to gas networks in [10, 56]. In [3] the maximization of free booked capacities is considered. As mentioned above, the TSO sells rights to inject and withdraw gas at certain points. These rights constitutes bounds for the nominations. Let I and W denote the booked capacities at the injection points and the withdrawal points, respectively, and q_+^{nom} and q_-^{nom} the nominations (loads) at the injection and withdrawal points, respectively. Then the TSO has to ensure that

$$\forall (q_+^{\text{nom}}, q_-^{\text{nom}}) : q_+^{\text{nom}} \in [-I, 0], q_-^{\text{nom}} \in [0, W], \\ (q_+^{\text{nom}}, q_-^{\text{nom}}) \text{ is a feasible load vector.}$$

Since for the nominations at the withdrawal points there exist historical data and their distribution can be estimated, this condition can be relaxed to

$$\mathbb{P} \left\{ q_-^{\text{nom}} \in [0, W] : (q_+^{\text{nom}}, q_-^{\text{nom}}) \text{ is a feasible load vector } \forall q_+^{\text{nom}} \in [-I, 0] \right\} \geq p,$$

where p is a prescribed probability level close to 1. If the probability on the left-hand side is strictly greater than the probability level p , the TSO can sell more capacities to maximize his profit. This optimization problem reads

$$\max \left\{ \mathbf{1}^T x_+ + \mathbf{1}^T x_- : \mathbb{P} \left\{ q_-^{\text{nom}} \in [0, W] : (q_+^{\text{nom}}, q_-^{\text{nom}} + y) \text{ is a feasible} \right. \right. \\ \left. \left. \text{load vector } \forall y \in [0, x_-] \forall q_+^{\text{nom}} \in [-I - x_+, 0] \right\} \geq p \right\}.$$

This emphasizes the importance of computing the probability of load vectors to be feasible.

This thesis focuses on problems with uncertain loads for which historical data are available leading to probabilistic constraints. This means that only the exit loads are considered random. The loads at the injection points are market driven and hence can not be approximated by a distribution. To avoid a robust consideration of the entry loads the networks in this thesis contain exactly one entry node. This singularity often appears in distribution networks. Let ξ be a random vector representing the exit loads, then the aim is to determine the probability

$$\mathbb{P} \{ \omega \in \Omega : \xi(\omega) \text{ is a feasible exit load vector} \}$$

of feasible exit load vectors. This question was already addressed in [57], but there only networks with at most one fundamental cycle were treated. As in [57], a reparametrization technique called spheric-radial decomposition, cf. [51], is used to tackle this probability. To be able to treat also networks with several fundamental cycles that are not edge-disjoint, Gröbner bases ([2, 31, 32]) are utilized to solve the polynomial systems occurring in the course of spheric-radial decomposition.

There already exist works on using Gröbner bases, nonparametric and parametric, in the load flow problem for electrical networks, see [47, 85, 86, 89]. However,

the approaches outlined there all have the same limitations: they can not deal with networks of practical size because the computations become too complex and consume a lot of computational resources. In the same way, even though Gröbner bases enable to tackle networks with several fundamental cycles that are not edge-disjoint, the method is limited to a small number of those fundamental cycles.

Parametric optimization problems arising in model predictive control are of high interest. Predictive model control solves optimal control problems by optimizing the current time step while keeping future time steps into account. Then the solution of the first time step is implemented and the problem is solved again for the next time step. The optimization problem reads as follows [45]:

$$\min_x f(x, u) \quad \text{s.t. } g_i(x, u) \leq 0 \quad \text{for } i = 1, \dots, t, \quad (1.1)$$

where $f, g_1, \dots, g_t \in k[u_1, \dots, u_m][x_1, \dots, x_n]$. Here, the function f is to be minimized with respect to the decision variable x for any given value of the parameter u . By [21] (Karush-Kuhn-Tucker optimality conditions) any minimum of this optimization problem is a solution of

$$\nabla_x f(x, u) + \sum_{i=1}^t \lambda_i \nabla_x g_i(x, u) = 0 \quad (1.2)$$

$$\lambda_i g_i(x, u) = 0 \quad \forall i = 1, \dots, t \quad (1.3)$$

$$\lambda_i \geq 0 \quad \forall i = 1, \dots, t \quad (1.4)$$

$$g_i(x, u) \leq 0 \quad \forall i = 1, \dots, t. \quad (1.5)$$

Equations (1.2) and (1.3) build a polynomial equation system with as many indeterminates as equations and it can be solved using Gröbner basis techniques.

To solve problem (1.1) one has to solve the polynomial equation system (1.2), (1.3), discard all solutions that are infeasible due to (1.4) and (1.5) and then search for the solution among the remaining solutions with minimal value under evaluation of f . The aim is to handle as much of the computational effort as possible before the parameter u is fixed. In optimization problems concerning gas networks this can be done by solving the feasibility problem of loads parametrically using comprehensive Gröbner systems.

This thesis is organized as follows. The first part is devoted to introductions on topics that are important for the research presented in this thesis. Chapter 2 deals with algebraic fundamentals needed to solve systems of polynomial equations. In this chapter, basis definitions are introduced as well as Gröbner bases and their applications. The chapter concludes with a short treatment of comprehensive Gröbner systems. Chapter 3 gives a very brief introduction to graphs and digraphs. In Chapter 4 the modeling of gas networks is outlined. First, the physical properties of gas and the gas flow along a single pipe are discussed. After that the modeling is extended to entire networks. In these preliminaries no proofs are contained in order not to blow up the length of this thesis.

In the main part of this thesis new research results are presented. In Chapter 5 the feasibility of loads is characterized. An algorithm to validate feasibility of a given load using Gröbner bases is stated. Moreover, some rules for possible flow directions along the pipes are given and an upper bound for the number of possible flow directions is deduced. Last, a method for finding redundant pressure bounds is given. In Chapter 6 the probability of exit loads to be feasible is examined. First, the theory is given and an algorithm to compute the probability involving Gröbner basis techniques in the course of spheric-radial decomposition is introduced. Afterwards, some numerical results are presented. The part concludes with a parametric consideration of the feasibility problem.

The appendix contains infeasible flow directions of some examples occurring in the thesis and data of some networks considered.

Parts of this thesis have been submitted for publication, see [58].

Part I
Preliminaries

Chapter 2

Solving Systems of Polynomial Equations

In the main part of this thesis one of the crucial tasks will be to find all solutions of systems of polynomial equations. This chapter will provide the method used and its algebraic background. First, in Section 2.1 terms such as polynomial, ideal, and variety are introduced. Gröbner bases will come into play in Section 2.2. Moreover, the way how Gröbner bases can be used to solve systems of polynomial equations is discussed there as well as some special settings where Gröbner bases exhibit an especially simple form, called Shape basis. In Section 2.3 comprehensive Gröbner systems are defined. They can be seen as parametric Gröbner bases for ideals where the polynomials depend not only on indeterminates but also on parameters.

Unless otherwise stated the content of this chapter can be found in [2, 31, 32]. These books are recommendable introductions into the field of polynomial algebra.

Although in the rest of this thesis vectors are always column vectors, in this chapter they are dealt with as rows for convenience and to simplify notation.

2.1 Introduction to Polynomials, Varieties, and Ideals

In this section the principal terms polynomial, variety, ideal, and radical ideal are introduced. Moreover, some of their properties and their interdependencies are explained.

Let k denote a field. In this thesis, k is always \mathbb{Q} , \mathbb{R} or \mathbb{C} .

A monomial in x_1, \dots, x_n is a product of the form $x_1^{\alpha_1} \cdots x_n^{\alpha_n}$ with $\alpha_1, \dots, \alpha_n \in \mathbb{Z}_{\geq 0}$. The total degree of this monomial is the sum $\text{totaldeg}(x_1^{\alpha_1} \cdots x_n^{\alpha_n}) := \alpha_1 + \cdots + \alpha_n$. With $\alpha = (\alpha_1, \dots, \alpha_n)$ the notation of a monomial can be simplified to $x^\alpha = x_1^{\alpha_1} \cdots x_n^{\alpha_n}$.

A polynomial f in x_1, \dots, x_n with coefficients in the field k is a finite linear

combination of monomials written

$$f = \sum_{\alpha} c_{\alpha} x^{\alpha}, \quad c_{\alpha} \in k.$$

The set of all polynomials over k is denoted $k[x_1, \dots, x_n]$. It is easily verified that $k[x_1, \dots, x_n]$ is a commutative ring.

A field is called algebraically closed if every nonconstant polynomial in $k[x]$ has a root in k . Hence, \mathbb{C} is algebraically closed whereas \mathbb{R} is not.

Let f be a polynomial as given in the above definition. Then c_{α} is called the coefficient of the monomial x^{α} and $c_{\alpha} x^{\alpha}$ is called term of f . The total degree of f is $\deg f := \max \{\text{totaldeg}(x^{\alpha}) : c_{\alpha} \neq 0\}$.

The set $k^n := \{(a_1, \dots, a_n) : a_1, \dots, a_n \in k\}$ denotes the n -dimensional affine space over k . Each polynomial $f = \sum_{\alpha} c_{\alpha} x^{\alpha} \in k[x_1, \dots, x_n]$ determines a function $f : k^n \rightarrow k$ defined $(b_1, \dots, b_n) \mapsto f(b_1, \dots, b_n) = \sum_{\alpha} c_{\alpha} b^{\alpha}$, known as evaluation of f on b . This is a common way to connect algebra and geometry.

Given some polynomials $f_1, \dots, f_s \in k[x_1, \dots, x_n]$, the purpose of this chapter is to determine the points a in the affine space k^n for which $f_1(a) = 0, \dots, f_s(a) = 0$. The set of all these points is called affine variety defined by the polynomials $f_1, \dots, f_s \in k[x_1, \dots, x_n]$,

$$\mathbf{V}(f_1, \dots, f_s) := \{(a_1, \dots, a_n) \in k^n : f_i(a_1, \dots, a_n) = 0 \text{ for all } i = 1, \dots, s\}.$$

A subset $\mathcal{I} \subseteq k[x_1, \dots, x_n]$ is an ideal if $0 \in \mathcal{I}$, if $f + g \in \mathcal{I}$ for $f, g \in \mathcal{I}$, and if $hf \in \mathcal{I}$ for $f \in \mathcal{I}$ and $h \in k[x_1, \dots, x_n]$.

Let $f_1, \dots, f_s \in k[x_1, \dots, x_n]$ be polynomials. The ideal generated by f_1, \dots, f_s is

$$\langle f_1, \dots, f_s \rangle := \left\{ \sum_{i=1}^s h_i f_i : h_1, \dots, h_s \in k[x_1, \dots, x_n] \right\}.$$

Indeed, for $f_1, \dots, f_s \in k[x_1, \dots, x_n]$, $\langle f_1, \dots, f_s \rangle$ is an ideal in $k[x_1, \dots, x_n]$ and the polynomials f_1, \dots, f_s build a basis for this ideal.

For an affine variety $\mathcal{V} \subseteq k^n$ the set

$$\mathbf{I}(\mathcal{V}) := \{f \in k[x_1, \dots, x_n] : f(a_1, \dots, a_n) = 0 \text{ for all } (a_1, \dots, a_n) \in \mathcal{V}\}$$

is an ideal, called the ideal of \mathcal{V} . If $f_1, \dots, f_s \in k[x_1, \dots, x_n]$ are polynomials, then $\langle f_1, \dots, f_s \rangle \subseteq \mathbf{I}(\mathbf{V}(f_1, \dots, f_s))$. The following small example shows that equality need not to occur. Consider the ideal $\mathcal{I} = \langle x^2, y^2 \rangle \subseteq k[x, y]$. Then $\mathbf{V}(x^2, y^2) = \{(0, 0)\}$, i.e., $x, y \in \mathbf{I}(\mathbf{V}(x^2, y^2))$, but $x, y \notin \mathcal{I}$.

Now, let $\mathcal{I} \subseteq k[x_1, \dots, x_n]$ be an ideal. Then the set

$$\mathbf{V}(\mathcal{I}) := \{(a_1, \dots, a_n) \in k^n : f(a_1, \dots, a_n) = 0 \text{ for all } f \in \mathcal{I}\}$$

is an affine variety. It is easily seen that $\mathbf{V}(\mathcal{I}) = \mathbf{V}(f_1, \dots, f_s)$ if the polynomials f_1, \dots, f_s generate the ideal \mathcal{I} . This leads to the following proposition.

Proposition 2.1. *Let f_1, \dots, f_s and g_1, \dots, g_t be polynomials in $k[x_1, \dots, x_n]$ that generate the same ideal \mathcal{I} . Then $\mathbf{V}(f_1, \dots, f_s) = \mathbf{V}(g_1, \dots, g_t)$.*

Hence, when solving a system of polynomials $f_1 = 0, \dots, f_s = 0$, the idea is to find another basis g_1, \dots, g_t for the ideal $\langle f_1, \dots, f_s \rangle$ such that the system of polynomials $g_1 = 0, \dots, g_t = 0$ is easier to solve. Remember that linear equations are polynomial equations. When solving a system of linear equations, Gaussian elimination is utilized to transfer the system into row reduced echelon form. The equations of the “new” system form a basis of the ideal generated by the equations of the original system, but are much easier to solve. The question under consideration now is, is there a way to perform such transformations on general systems of polynomial equations and not just on linear systems? The answer is yes as will be seen in Section 2.2 about Gröbner bases.

If an ideal \mathcal{I} in $k[x_1, \dots, x_n]$ contains the constant polynomial 1, and hence $\mathcal{I} = k[x_1, \dots, x_n]$, then the variety $\mathbf{V}(\mathcal{I})$ is empty. If k is algebraically closed, equivalency holds as the next theorem states.

Theorem 2.2 (Weak Nullstellensatz). *Let k be an algebraically closed field and \mathcal{I} an ideal in $k[x_1, \dots, x_n]$. If $\mathbf{V}(\mathcal{I}) = \emptyset$, then $\mathcal{I} = k[x_1, \dots, x_n]$.*

To see why the Weak Nullstellensatz does not hold for arbitrary fields consider the ideal $\mathcal{I} = \langle x^2 + 1 \rangle$ in $\mathbb{R}[x]$. Then $\mathbf{V}(\mathcal{I}) = \emptyset$ although $1 \notin \mathcal{I}$.

Since $\mathbf{V}(\mathbf{I}(\mathcal{V})) = \mathcal{V}$ for all affine varieties $\mathcal{V} \subseteq k^n$, the map

$$\mathbf{I}: \text{affine varieties} \rightarrow \text{ideals}$$

is one-to-one. On the contrary, it can happen that two distinct ideals define the same affine variety. For instance, 0 is the only root of the polynomials x and x^2 , no matter which field is considered. Thus $\mathbf{V}(\langle x \rangle) = \mathbf{V}(\langle x^2 \rangle)$. It follows that the map

$$\mathbf{V}: \text{ideals} \rightarrow \text{affine varieties}$$

is not one-to-one.

The main reason why distinct ideals can define the same affine variety is that a polynomial f and any power f^m for an arbitrary integer $m \geq 1$ have exactly the same roots: Let $f, f_1, \dots, f_s \in k[x_1, \dots, x_n]$ be polynomials and $m \geq 1$ an integer. If $f^m \in \langle f_1, \dots, f_s \rangle$, then $f \in \mathbf{I}(\mathbf{V}(\langle f_1, \dots, f_s \rangle))$. Thus, if in addition $f \notin \langle f_1, \dots, f_s \rangle$, then $\langle f_1, \dots, f_s \rangle$ and $\langle f_1, \dots, f_s, f \rangle$ are distinct ideals with $\mathbf{V}(\langle f_1, \dots, f_s \rangle) = \mathbf{V}(\langle f_1, \dots, f_s, f \rangle)$.

The assertion of the following theorem is, that if the underlying field is algebraically closed, then this is the only reason why this can happen.

Theorem 2.3 (Hilbert’s Nullstellensatz). *Let k be an algebraically closed field and $f, f_1, \dots, f_s \in k[x_1, \dots, x_n]$ polynomials. If $f \in \mathbf{I}(\mathbf{V}(f_1, \dots, f_s))$, then there exists an integer $m \geq 1$ such that $f^m \in \langle f_1, \dots, f_s \rangle$.*

This motivates the definition of radical ideals. A polynomial ideal \mathcal{I} is called radical if $f \in \mathcal{I}$ whenever $f^m \in \mathcal{I}$ for some integer $m \geq 1$.

As an example, let \mathcal{V} be an affine variety. Then the ideal $\mathbf{I}(\mathcal{V})$ of \mathcal{V} is radical. Let \mathcal{I} be an ideal in $k[x_1, \dots, x_n]$. Then the radical of \mathcal{I} is the set

$$\sqrt{\mathcal{I}} := \{f : f^m \in \mathcal{I} \text{ for some } m \in \mathbb{Z}, m \geq 1\}.$$

It follows that an ideal \mathcal{I} is radical if and only if $\mathcal{I} = \sqrt{\mathcal{I}}$ holds. Moreover, $\sqrt{\mathcal{I}}$ is a radical ideal in $k[x_1, \dots, x_n]$ with $\mathcal{I} \subseteq \sqrt{\mathcal{I}}$.

With this notation, Hilbert's Nullstellensatz 2.3 can be reformulated.

Theorem 2.4 (Strong Nullstellensatz). *Let k be an algebraically closed field and \mathcal{I} an ideal in $k[x_1, \dots, x_n]$. Then $\mathbf{I}(\mathbf{V}(\mathcal{I})) = \sqrt{\mathcal{I}}$.*

This yields that $\mathbf{I}(\mathbf{V}(\mathcal{I})) = \mathcal{I}$ if and only if \mathcal{I} is radical. Assuming that k is an algebraically closed field, this implies that the maps

$$\mathbf{I}: \text{affine varieties} \rightarrow \text{radical ideals}$$

and

$$\mathbf{V}: \text{radical ideals} \rightarrow \text{affine varieties}$$

are inverses of each other and thus bijections.

2.2 Gröbner Bases and Applications

This section is devoted to the bases of an ideal that simplify the underlying system of polynomial equations, called Gröbner bases. Gröbner bases were introduced in 1965 by Bruno Buchberger in his dissertation [22] and received their name in 1976 in Buchberger's paper [23]. Whilst Buchberger devoted the bases to the supervisor of his dissertation, Wolfgang Gröbner, the algorithm to compute them is named after him. The concept of Gröbner bases was already introduced in [62] in 1964 by Hironaka. However, Hironaka's proof of existence was not constructive and he did not give an algorithm to compute them.

To compute a Gröbner basis an algorithm to divide a polynomial by other polynomials is needed. This algorithm is given in Subsection 2.2.2. The definition of Gröbner bases is introduced in Subsection 2.2.4 and some nice properties of Gröbner bases are listed in Subsubsection 2.2.4.2. For instance, Gröbner bases enable to decide if a given polynomial lies in a given ideal or not. In Subsubsection 2.2.4.3 an algorithm to compute Gröbner bases is discussed.

Subsection 2.2.5 shows how Gröbner bases can be used to solve systems of polynomial equations and in Subsection 2.2.6 the Shape Lemma, a lemma stating under which conditions the reduced Gröbner basis w.r.t. the lexicographic ordering has an even easier to solve structure, is introduced.

2.2.1 Monomial Orderings

For the following considerations, the monomials of a polynomial must be ordered in some way.

Since every monomial $x_1^{\alpha_1} \cdots x_n^{\alpha_n}$ can be written in the form x^α with $\alpha \in \mathbb{Z}_{\geq 0}^n$ and every $\alpha \in \mathbb{Z}_{\geq 0}^n$ yields the monomial x^α in $k[x_1, \dots, x_n]$, there is a one-to-one correspondence between the monomials in $k[x_1, \dots, x_n]$ and $\mathbb{Z}_{\geq 0}^n$. With an ordering \succ on $\mathbb{Z}_{\geq 0}^n$ given, the monomials can be ordered according to the following rule:

$$\alpha \succ \beta \iff x^\alpha \succ x^\beta.$$

These orderings have to meet some requirements.

Definition 2.5 (Monomial Ordering). A monomial ordering \succeq on $k[x_1, \dots, x_n]$ is a relation \succeq on $\mathbb{Z}_{\geq 0}^n$ or equivalent a relation on the set of monomials x^α , $\alpha \in \mathbb{Z}_{\geq 0}^n$, that fulfills the following three conditions:

- (i) \succeq is a total ordering on $\mathbb{Z}_{\geq 0}^n$.
- (ii) If $\alpha \succeq \beta$ and $\gamma \in \mathbb{Z}_{\geq 0}^n$, then $\alpha + \gamma \succeq \beta + \gamma$.
- (iii) \succeq is a well-ordering on $\mathbb{Z}_{\geq 0}^n$, i.e., every nonempty subset of $\mathbb{Z}_{\geq 0}^n$ has a smallest element under \succeq .

Let \succ be a relation on the set of monomials. Then $x^\alpha \succ x^\beta$ if and only if $x^\alpha \succeq x^\beta$ and $x^\alpha \neq x^\beta$.

Lemma 2.6. An ordering \succeq on $\mathbb{Z}_{\geq 0}^n$ is a well-ordering if and only if every strictly decreasing sequence

$$\alpha_1 \succ \alpha_2 \succ \alpha_3 \succ \cdots$$

in $\mathbb{Z}_{\geq 0}^n$ terminates.

It is easily seen that the following three relations are monomial orderings. All of these monomial orderings have their own advantages and disadvantages and the choice of the monomial ordering should be considered carefully. Later, this will be discussed in more detail.

Definition 2.7 (Lexicographic Ordering). Let $\alpha, \beta \in \mathbb{Z}_{\geq 0}^n$. Then $\alpha \succ_{lex} \beta$ if the first nonzero entry of $\alpha - \beta$ is positive. Furthermore, $x^\alpha \succ_{lex} x^\beta$ if $\alpha \succ_{lex} \beta$.

Definition 2.8 (Graded Lexicographic Ordering). Let $\alpha, \beta \in \mathbb{Z}_{\geq 0}^n$. Then $\alpha \succ_{grlex} \beta$ if

$$\text{totaldeg}(x^\alpha) > \text{totaldeg}(x^\beta)$$

or

$$\text{totaldeg}(x^\alpha) = \text{totaldeg}(x^\beta) \quad \text{and} \quad \alpha \succ_{lex} \beta.$$

Definition 2.9 (Graded Reverse Lexicographic Ordering). Let $\alpha, \beta \in \mathbb{Z}_{\geq 0}^n$. Then $\alpha \succ_{\text{grevlex}} \beta$ if

$$\text{totaldeg}(x^\alpha) > \text{totaldeg}(x^\beta)$$

or

$$\text{totaldeg}(x^\alpha) = \text{totaldeg}(x^\beta) \quad \text{and the last nonzero entry of } \alpha - \beta \text{ is negative.}$$

Let $f = \sum_{\alpha} c_{\alpha} x^{\alpha} \neq 0$ be a polynomial in $k[x_1, \dots, x_n]$ and \succeq a monomial ordering. Then $\text{multideg}(f) := \max \{ \alpha \in \mathbb{Z}_{\geq 0}^n : c_{\alpha} \neq 0 \}$ denotes the multidegree of f , $\text{lc}(f) := c_{\text{multideg}(f)} \in k$ denotes the leading coefficient of f , $\text{lm}(f) := x^{\text{multideg}(f)}$ denotes the leading monomial of f , and $\text{lt}(f) := \text{lc}(f) \cdot \text{lm}(f)$ denotes the leading term of f .

If $f, g \neq 0$ are polynomials in $k[x_1, \dots, x_n]$, it is easily seen that $\text{multideg}(fg) = \text{multideg}(f) + \text{multideg}(g)$. Furthermore, if $f + g \neq 0$ then

$$\text{multideg}(f + g) \preceq \max \{ \text{multideg}(f), \text{multideg}(g) \}.$$

If in addition $\text{multideg}(f) \neq \text{multideg}(g)$, equality occurs.

Let k be a field and \mathcal{I} an ideal in the polynomial ring $k[x]$ of polynomials in one indeterminate. Then $\mathcal{I} = \langle f \rangle$ for some polynomial $f \in k[x]$ with minimal degree. Moreover, f is uniquely determined up to multiplication by a nonzero constant in k . A ring with this property is called principal ideal ring.

2.2.2 A Division Algorithm in $k[x_1, \dots, x_n]$

In this subsection an algorithm for dividing a polynomial f by polynomials f_1, \dots, f_s is discussed.

Algorithm 2.10 (Division Algorithm).

Input: Polynomials f_1, \dots, f_s, f , monomial ordering \succeq

Output: Polynomials h_1, \dots, h_s, r such that $f = h_1 f_1 + \dots + h_s f_s + r$

$h_1 := 0, \dots, h_s := 0, r := 0$

$p := f$

WHILE $p \neq 0$ DO

$i := 1$

 divisionoccurred := False

 WHILE $i \leq s$ AND divisionoccurred = False DO

 IF $\text{lt}(p)$ is divisible by $\text{lt}(f_i)$ THEN

$h_i := h_i + \text{lt}(p) / \text{lt}(f_i)$

$p := p - (\text{lt}(p) / \text{lt}(f_i)) f_i$

 divisionoccurred := True

 ELSE

```

      i := i + 1
    IF division occurred = False THEN
      r := r + lt(p)
      p := p - lt(p)
    RETURN h1, ..., hs, r

```

Proposition 2.11. *Let \succeq be a monomial ordering on $\mathbb{Z}_{\geq 0}^n$ and $F = (f_1, \dots, f_s)$ an ordered s -tuple of polynomials in $k[x_1, \dots, x_n]$. Then by applying Algorithm 2.10 every polynomial $f \in k[x_1, \dots, x_n]$ can be written in the form*

$$f = h_1 f_1 + \dots + h_s f_s + r, \quad h_1, \dots, h_s, r \in k[x_1, \dots, x_n] \quad (2.1)$$

such that either r is the zero polynomial or r is a linear combination in k of monomials, none of which is divisible by any of $\text{lt}(f_1), \dots, \text{lt}(f_s)$. The polynomial r is called the remainder on division of f by F , denoted $r_F(f)$. Moreover, if $h_i f_i \neq 0$, then $\text{multideg}(f) \succeq \text{multideg}(h_i f_i)$.

Consider the polynomials $f_1 = xy + 1, f_2 = y^2 - 1, f = xy^2 - x \in k[x, y]$ equipped with the lexicographic ordering. If Division Algorithm 2.10 is used to divide f by the 2-tuple $F = (f_1, f_2)$, then the representation

$$xy^2 - x = y(xy + 1) + 0(y^2 - 1) + (-x - y)$$

is obtained. If, on the contrary, f is divided by the 2-tuple $F = (f_2, f_1)$, then the result is

$$xy^2 - x = x(y^2 - 1) + 0(xy + 1) + 0.$$

This example shows that h_1, \dots, h_s and r depend on the order of f_1, \dots, f_s . Furthermore, a polynomial f can be an element of the ideal generated by f_1, \dots, f_s although the remainder on division of f by f_1, \dots, f_s is not equal to zero. Hence, the condition $r = 0$ is sufficient for $f \in \langle f_1, \dots, f_s \rangle$, but not necessary.

Thus, a desirable property of a basis of an ideal is that the remainder on division by this basis is independent of the order of the generators. Then $r = 0$ is equivalent to f being in this ideal. In Subsection 2.2.4 a basis will be introduced that fulfills this property.

2.2.3 Dickson's Lemma

Definition 2.12 (Monomial Ideal). An ideal $\mathcal{I} \subseteq k[x_1, \dots, x_n]$ is called a monomial ideal if there exists a, possibly infinite, subset $A \subseteq \mathbb{Z}_{\geq 0}^n$ such that \mathcal{I} consists of all finite sums of the form

$$\sum_{\alpha \in A} h_{\alpha} x^{\alpha} \in k[x_1, \dots, x_n], \quad h_{\alpha} \in k[x_1, \dots, x_n] \text{ for all } \alpha \in A,$$

denoted $\mathcal{I} = \langle x^{\alpha} : \alpha \in A \rangle$.

Lemma 2.13. *Let $\mathcal{I} = \langle x^\alpha : \alpha \in A \rangle$ be a monomial ideal. Then a monomial x^β is an element of \mathcal{I} if and only if x^β is divisible by some x^α with $\alpha \in A$.*

The monomial x^β is divisible by x^α if and only if $x^\beta = x^\alpha x^\gamma$ for $\gamma \in \mathbb{Z}_{\geq 0}^n$ which is equivalent to $\beta = \alpha + \gamma$. Thus the set of all monomials that are divisible by x^α is given by

$$\alpha + \mathbb{Z}_{\geq 0}^n := \{ \alpha + \gamma : \gamma \in \mathbb{Z}_{\geq 0}^n \}.$$

Let \mathcal{I} be a monomial ideal and $f \in k[x_1, \dots, x_n]$ a polynomial. Then $f \in \mathcal{I}$ if and only if each term of f lies in \mathcal{I} . And this is the case if and only if f is a linear combination of monomials in \mathcal{I} with coefficients in k .

As a consequence, two monomial ideals coincide if and only if they contain the same monomials. Hence, a monomial ideal is uniquely determined by its monomials.

The next proposition states that every monomial ideal has a finite generating set.

Proposition 2.14 (Dickson's Lemma). *Let $\mathcal{I} = \langle x^\alpha : \alpha \in A \rangle$ be a monomial ideal. Then \mathcal{I} can be represented in the form*

$$\mathcal{I} = \langle x^{\alpha_1}, \dots, x^{\alpha_s} \rangle, \quad \alpha_1, \dots, \alpha_s \in A.$$

Hence, \mathcal{I} has a finite basis.

2.2.4 Gröbner Bases

2.2.4.1 Definition of Gröbner Bases

Let $\mathcal{I} \neq \{0\}$ be an ideal in $k[x_1, \dots, x_n]$. Then

$$\text{lt}(\mathcal{I}) := \{ cx^\alpha : \exists f \in \mathcal{I} \text{ with } \text{lt}(f) = cx^\alpha \}$$

is the set of leading terms of elements of \mathcal{I} and $\langle \text{lt}(\mathcal{I}) \rangle$ is the ideal generated by the elements of $\text{lt}(\mathcal{I})$.

If $\mathcal{I} = \langle f_1, \dots, f_s \rangle$, then $\langle \text{lt}(f_1), \dots, \text{lt}(f_s) \rangle \subseteq \langle \text{lt}(\mathcal{I}) \rangle$, because $\{ \text{lt}(f_1), \dots, \text{lt}(f_s) \} \subseteq \text{lt}(\mathcal{I})$. But $\langle \text{lt}(\mathcal{I}) \rangle$ can be strictly larger, as the following example shows.

Consider the polynomial ring $k[x, y]$ equipped with the graded lexicographic ordering and set $f_1 = x^3 - 2xy$ and $f_2 = x^2y - 2y^2 + x$. Then $x^2 = -yf_1 + xf_2 \in \mathcal{I} := \langle f_1, f_2 \rangle$ and hence $x^2 = \text{lt}(x^2) \in \langle \text{lt}(\mathcal{I}) \rangle$. However, x^2 is neither divisible by $\text{lt}(f_1) = x^3$ nor by $\text{lt}(f_2) = x^2y$, thus $x^2 \notin \langle \text{lt}(f_1), \text{lt}(f_2) \rangle$ by Lemma 2.13.

Lemma 2.15. *Let $\mathcal{I} \subseteq k[x_1, \dots, x_n]$ be an ideal. Then it holds:*

(i) $\langle \text{lt}(\mathcal{I}) \rangle$ is a monomial ideal.

(ii) There exist $g_1, \dots, g_t \in \mathcal{I}$ such that $\langle \text{lt}(\mathcal{I}) \rangle = \langle \text{lt}(g_1), \dots, \text{lt}(g_t) \rangle$.

Theorem 2.16 (Hilbert Basis Theorem). *For every ideal $\mathcal{I} \subseteq k[x_1, \dots, x_n]$ there are finitely many $g_1, \dots, g_t \in \mathcal{I}$, such that $\mathcal{I} = \langle g_1, \dots, g_t \rangle$. Hence, every ideal has a finite generating set.*

Let $f_1, \dots, f_s \in k[x_1, \dots, x_n]$ be polynomials and \mathcal{I} the ideal generated by these polynomials. Denote $F = (f_1, \dots, f_s)$ and consider a polynomial $f \in \mathcal{I}$. Subsection 2.2.2 contains an example that shows that the remainder $r_F(f)$ need not to be zero in that case (however, $r_F(f) = 0$ implies $f \in \mathcal{I}$). From representation (2.1) it follows that $r_F(f) \in \mathcal{I}$. Moreover, its terms are not divisible by the leading terms of the elements of F because otherwise the particular term would not belong to the remainder on division of f by F . To ensure that the remainder on division of all elements of \mathcal{I} by the generators of \mathcal{I} are zero, the leading terms of all elements of \mathcal{I} have to be divisible by the leading term of one of the generators of \mathcal{I} . This motivates the definition of Gröbner bases.

Definition 2.17 (Gröbner Basis). A finite subset $\mathcal{G} = \{g_1, \dots, g_t\}$ of an ideal \mathcal{I} is called Gröbner basis if

$$\langle \text{lt}(g_1), \dots, \text{lt}(g_t) \rangle = \langle \text{lt}(\mathcal{I}) \rangle$$

holds.

Lemma 2.13 and the comments thereafter yield this equivalent formulation of the definition of Gröbner bases: $\{g_1, \dots, g_t\} \subseteq \mathcal{I}$ is a Gröbner basis of \mathcal{I} if and only if the leading term of every element in \mathcal{I} is divisible by any $\text{lt}(g_1), \dots, \text{lt}(g_t)$.

Corollary 2.18. *Every ideal $\mathcal{I} \neq \{0\}$ in $k[x_1, \dots, x_n]$ has a Gröbner basis. Moreover, every Gröbner basis of an ideal \mathcal{I} is a basis of \mathcal{I} , i.e., \mathcal{I} is generated by the elements of its Gröbner basis.*

2.2.4.2 Properties of Gröbner Bases

Proposition 2.19. *Let \mathcal{I} be an ideal in $k[x_1, \dots, x_n]$, $\mathcal{G} = \{g_1, \dots, g_t\}$ a Gröbner basis of \mathcal{I} and $f \in k[x_1, \dots, x_n]$ a polynomial. Then there exists a uniquely determined $r \in k[x_1, \dots, x_n]$ such that the following holds:*

- (i) *No term of r is divisible by any of $\text{lt}(g_1), \dots, \text{lt}(g_t)$.*
- (ii) *There exists $g \in \mathcal{I}$ such that $f = g + r$.*

r is the remainder on division of f by \mathcal{G} . Moreover, r does not depend on the order of the g_i in \mathcal{G} .

Corollary 2.20. *Let \mathcal{I} be an ideal in $k[x_1, \dots, x_n]$, $\mathcal{G} = \{g_1, \dots, g_t\}$ a Gröbner basis of \mathcal{I} and $f \in k[x_1, \dots, x_n]$ a polynomial. Then $f \in \mathcal{I}$ if and only if the remainder on division of f by \mathcal{G} is zero.*

Corollary 2.20 gives an easy to check criterion to decide whether a given polynomial lies in an ideal or not.

Definition 2.21 (*S*-Polynomial). Let $f, g \in k[x_1, \dots, x_n] \setminus \{0\}$ be polynomials.

(i) Set $\text{multideg}(f) := \alpha$ and $\text{multideg}(g) := \beta$. If $\gamma = (\gamma_1, \dots, \gamma_n)$ where $\gamma_i := \max\{\alpha_i, \beta_i\}$ for all $i = 1, \dots, n$, then x^γ is called the least common multiple of $\text{lm}(f)$ and $\text{lm}(g)$ denoted $\text{lcm}(\text{lm}(f), \text{lm}(g))$.

(ii) The *S*-polynomial of f and g is

$$S(f, g) := \frac{x^\gamma}{\text{lt}(f)}f - \frac{x^\gamma}{\text{lt}(g)}g,$$

where $x^\gamma = \text{lcm}(\text{lm}(f), \text{lm}(g))$.

The following criterion makes a crucial contribution to the algorithm for the computation of a Gröbner basis.

Theorem 2.22 (Buchberger's Criterion). *Let \mathcal{I} be a polynomial ideal. Then a basis $\mathcal{G} = \{g_1, \dots, g_t\}$ is a Gröbner basis of \mathcal{I} if and only if the remainder on division of $S(g_i, g_j)$ by \mathcal{G} equals zero for all pairs $i, j \in \{1, \dots, t\}$ with $i \neq j$.*

2.2.4.3 Buchberger's Algorithm

Now, every component needed to formulate an algorithm for the computation of a Gröbner basis is available.

Algorithm 2.23 (Buchberger's Algorithm).

Input: $F = \{f_1, \dots, f_s\}$ with $f_1, \dots, f_s \in k[x_1, \dots, x_n]$

Output: Gröbner basis \mathcal{G} of $\mathcal{I} = \langle f_1, \dots, f_s \rangle$

$\mathcal{G} := F$

REPEAT

$\mathcal{G}' := \mathcal{G}$

 FOR each pair $\{p, q\}$, $p \neq q$, in \mathcal{G}' DO

$S := r_{\mathcal{G}'}(S(p, q))$

 IF $S \neq 0$ THEN

$\mathcal{G} := \mathcal{G} \cup \{S\}$

UNTIL $\mathcal{G} = \mathcal{G}'$

RETURN \mathcal{G}

Proposition 2.24. *Let $\mathcal{I} = \langle f_1, \dots, f_s \rangle \neq \{0\}$ be a polynomial ideal. Then Buchberger's Algorithm 2.23 computes in finitely many steps a Gröbner basis \mathcal{G} of \mathcal{I} with $\{f_1, \dots, f_s\} \subseteq \mathcal{G}$.*

It has to be mentioned that this algorithm is very rudimentary. An overview on how Buchberger's Algorithm can be improved can be found in [31, §9]. From the references therein, [49] and [55] have to be pointed out separately.

It can be shown that the number of computations needed in the course of Buchberger's Algorithm 2.23 is minimal if the graded reverse lexicographic ordering is used. Moreover, in this case the coefficients of the polynomials in the Gröbner basis are smaller than with other monomial orderings. However, the next subsection shows that the lexicographic ordering brings another benefit.

Lemma 2.25. *Let \mathcal{G} be a Gröbner basis of the polynomial ideal \mathcal{I} and $p \in \mathcal{G}$ a polynomial such that $\text{lt}(p) \in \langle \text{lt}(\mathcal{G} \setminus \{p\}) \rangle$. Then $\mathcal{G} \setminus \{p\}$ is a Gröbner basis of \mathcal{I} as well.*

Definition 2.26 (Minimal Gröbner Basis). A minimal Gröbner basis of a polynomial ideal \mathcal{I} is a Gröbner basis \mathcal{G} of \mathcal{I} such that

- (i) $\text{lc}(p) = 1$ for all $p \in \mathcal{G}$.
- (ii) $\text{lt}(p) \notin \langle \text{lt}(\mathcal{G} \setminus \{p\}) \rangle$ for all $p \in \mathcal{G}$.

Definition 2.27 (Reduced Gröbner Basis). A reduced Gröbner basis of a polynomial ideal \mathcal{I} is a Gröbner basis \mathcal{G} of \mathcal{I} such that

- (i) $\text{lc}(p) = 1$ for all $p \in \mathcal{G}$.
- (ii) For all $p \in \mathcal{G}$ it holds that no monomial of p lies in $\langle \text{lt}(\mathcal{G} \setminus \{p\}) \rangle$.

Theorem 2.28. *Let $\mathcal{I} \neq \{0\}$ be a polynomial ideal. Then \mathcal{I} has a uniquely determined reduced Gröbner basis.*

Uniqueness of the reduced Gröbner basis gives rise to the following equivalence: Two nontrivial ideals are the same if and only if their reduced Gröbner bases are the same.

The reduced Gröbner basis of an ideal can be computed from a Gröbner basis using the following algorithm.

Algorithm 2.29.

Input: Gröbner basis \mathcal{G} of a polynomial ideal \mathcal{I}

Output: Reduced Gröbner basis of \mathcal{I}

```

FOR each  $g \in \mathcal{G}$  DO
   $g := 1/\text{lc}(g) \cdot g$ 
FOR each  $g \in \mathcal{G}$  DO
  IF  $\text{lt}(g) \in \langle \text{lt}(\mathcal{G} \setminus \{g\}) \rangle$  THEN
     $\mathcal{G} := \mathcal{G} \setminus \{g\}$ 
FOR each  $g \in \mathcal{G}$  DO
   $g := r_{\mathcal{G} \setminus \{g\}}(g)$ 
RETURN  $\mathcal{G}$ 

```

2.2.5 Solving Systems of Polynomial Equations Using Gröbner Bases

Given a system of polynomial equations $f_1 = 0, \dots, f_s = 0$ with $f_1, \dots, f_s \in k[x_1, \dots, x_n]$, it was already pointed out that the varieties $\mathbf{V}(f_1, \dots, f_s)$ and $\mathbf{V}(\langle f_1, \dots, f_s \rangle)$ coincide. Aiming to find solutions of the system one would try to find consequences, i.e. multiplication by a polynomial in $k[x_1, \dots, x_n]$ and addition of two equations, of the equations $f_1 = 0, \dots, f_s = 0$ that eliminate the indeterminates one after the other, solve the “last” equation in only one indeterminate, and start a back-substitution process to find all solutions. For all the consequences $p = 0$ of the equations $f_1 = 0, \dots, f_s = 0$, the polynomial p is an element of the ideal $\langle f_1, \dots, f_s \rangle$. This gives rise to the following definition.

Definition 2.30. Let $\mathcal{I} = \langle f_1, \dots, f_s \rangle$ be an ideal in $k[x_1, \dots, x_n]$. Then the l -th elimination ideal $\mathcal{I}_l \subseteq k[x_{l+1}, \dots, x_n]$ is the ideal defined

$$\mathcal{I}_l := \mathcal{I} \cap k[x_{l+1}, \dots, x_n].$$

Given some polynomials $f_1, \dots, f_s \in k[x_1, \dots, x_n]$, the l -th elimination ideal \mathcal{I}_l consists of all consequences of the equations of the system $f_1 = 0, \dots, f_s = 0$ which eliminate the variables x_1, \dots, x_l . Now, the task is to find a basis for these ideals.

Theorem 2.31 (Elimination Theorem). *Let \mathcal{G} be a Gröbner basis of an ideal $\mathcal{I} \subseteq k[x_1, \dots, x_n]$ w.r.t. the lexicographic ordering with $x_1 \succ \dots \succ x_n$. Then $\mathcal{G}_l := \mathcal{G} \cap k[x_{l+1}, \dots, x_n]$ is a Gröbner basis of the l -th elimination ideal \mathcal{I}_l for every $l = 1, \dots, n - 1$.*

Elimination Theorem 2.31 states that $g_1 = 0, \dots, g_t = 0$, where $\mathcal{G} = \{g_1, \dots, g_t\}$ is a Gröbner basis of the ideal $\mathcal{I} = \langle f_1, \dots, f_s \rangle$ w.r.t. the lexicographic ordering with $x_1 \succ \dots \succ x_n$, is a representation of the system $f_1 = 0, \dots, f_s = 0$ that eliminates the indeterminate x_1 first, x_2 second, and so on. Moreover, if \mathcal{G}_{n-1} is nonempty, which is the case if the affine variety of \mathcal{I} is a finite set, then $\mathcal{G}_{n-1} = \{g\}$ for some $g \in k[x_n]$ because $k[x_n]$ is a principal ideal ring. Since every polynomial that eliminates x_1, \dots, x_{n-1} lies in \mathcal{I}_{n-1} and thus is a multiple of g , g is the best way to eliminate x_1, \dots, x_{n-1} .

For $l = 1, \dots, n - 1$, a solution $(a_{l+1}, \dots, a_n) \in \mathbf{V}(\mathcal{I}_l)$ is called partial solution of the original system of equations. If for some fixed $l \in \{1, \dots, n - 1\}$ such a partial solution $(a_{l+1}, \dots, a_n) \in \mathbf{V}(\mathcal{I}_l)$ is known, $a_l \in k$ with $(a_l, a_{l+1}, \dots, a_n) \in \mathbf{V}(\mathcal{I}_{l-1})$ has to be found. To do so, assume $\mathcal{I}_{l-1} = \langle g_1, \dots, g_t \rangle$. Then (a_{l+1}, \dots, a_n) is inserted into these polynomials and the system

$$g_1(x_l, a_{l+1}, \dots, a_n) = 0, \dots, g_t(x_l, a_{l+1}, \dots, a_n) = 0$$

is obtained. This is a system in only one indeterminate, namely x_l . But, these equations need not to have a common zero $a_l \in k$ as the following small example shows.

Consider the ideal $\mathcal{I} = \langle xz - 1, y - z \rangle \in \mathbb{C}[x, y, z]$. These polynomials form a Gröbner basis of the ideal and thus Elimination Theorem 2.31 can be applied. The equation $y - z = 0$ implies that (a, a) lies in $\mathbf{V}(\mathcal{I}_1)$ for all $a \in \mathbb{C}$. However, the partial solution $(0, 0)$ yields the equation $0 - 1 = 0$. Hence, $(0, 0)$ cannot be extended to a solution of the original system.

The next theorem makes it possible to decide in advance whether a partial solution can be extended or not.

Theorem 2.32 (Extension Theorem). *Let k be an algebraically closed field. Let $\mathcal{I} = \langle f_1, \dots, f_s \rangle$ be an ideal in $k[x_1, \dots, x_n]$ and \mathcal{I}_1 the first elimination ideal of \mathcal{I} . For every $i = 1, \dots, s$ let f_i be represented in the form*

$$f_i = g_i(x_2, \dots, x_n) x_1^{N_i} + \text{terms in which } x_1 \text{ has degree } < N_i,$$

where $N_i \geq 0$ and $0 \neq g_i \in k[x_2, \dots, x_n]$. Assume that a partial solution $(a_2, \dots, a_n) \in \mathbf{V}(\mathcal{I}_1)$ is given. If $(a_2, \dots, a_n) \notin \mathbf{V}(g_1, \dots, g_s)$, then there exists $a_1 \in k$ such that $(a_1, a_2, \dots, a_n) \in \mathbf{V}(\mathcal{I})$.

Two remarks are due. First, even though Extension Theorem 2.32 is formulated only in the case a partial solution of the first elimination ideal has to be extended to a full solution of the original system, it can be used to extend partial solutions of an arbitrary elimination ideal. To see why, note that \mathcal{I}_l is the first elimination ideal of \mathcal{I}_{l-1} for each $l = 1, \dots, n - 1$.

Second, the condition that k is an algebraically closed field is necessary. Consider the ideal $\langle x^2 - y, y - z \rangle \in \mathbb{R}[x, y, z]$. These polynomials form a Gröbner basis of the ideal. The equation $y - z = 0$ implies that (a, a) lies in $\mathbf{V}(\mathcal{I}_1)$ for all $a \in \mathbb{R}$. The constant $g_1(y, z) = 1$ does not vanish for any of the partial solutions, i.e., $(a, a) \notin \mathbf{V}(g_1)$ for all $a \in \mathbb{R}$. Yet, the partial solution (a, a) yields the equation $x^2 - a = 0$, that has no solution in \mathbb{R} whenever $a < 0$. Hence, in this case (a, a) cannot be extended to a solution of the original system.

Corollary 2.33. *Let k be an algebraically closed field, $\mathcal{I} = \langle f_1, \dots, f_s \rangle$ an ideal in $k[x_1, \dots, x_n]$, and \mathcal{I}_1 the first elimination ideal of \mathcal{I} . Suppose, there is some $i \in \{1, \dots, s\}$ such that f_i can be represented in the form*

$$f_i = \alpha x_1^N + \text{terms in which } x_1 \text{ has degree } < N,$$

where $N \geq 0$ and $0 \neq \alpha \in k$. Assume that a partial solution $(a_2, \dots, a_n) \in \mathbf{V}(\mathcal{I}_1)$ is given. Then there exists $a_1 \in k$ such that $(a_1, a_2, \dots, a_n) \in \mathbf{V}(\mathcal{I})$.

The preceding discussion indicates that Gröbner bases w.r.t. the lexicographic ordering reduce the problem of solving a system of multivariate polynomials to solving univariate polynomials. The roots of a univariate polynomial whose degree is not greater than 5 can be expressed as functions in the coefficients that use only the operations addition, subtraction, multiplication, and root extraction. For polynomials with higher degree, numerical methods have to be used. In general this could be Newton's methods, or, more suitable for polynomials, Laguerre's method (see, e.g., [1, 25]).

2.2.6 Shape Lemma

In some special cases the reduced Gröbner bases reveal an even better structure. For the formulation of these cases the concept of a quotient of a polynomial ring modulo an ideal has to be introduced. Moreover, some results concerning the Krull dimension of a ring are needed.

2.2.6.1 Quotient of a Polynomial Ring Modulo an Ideal

Let \mathcal{I} be an ideal in $k[x_1, \dots, x_n]$ and $f, g \in k[x_1, \dots, x_n]$ polynomials. Then f and g are congruent modulo \mathcal{I} , denoted

$$f \equiv g \pmod{\mathcal{I}},$$

if $f - g \in \mathcal{I}$. Congruency modulo \mathcal{I} is an equivalence relation on $k[x_1, \dots, x_n]$ with equivalence classes

$$\begin{aligned} [f] &:= \{g \in k[x_1, \dots, x_n] : g \equiv f \pmod{\mathcal{I}}\} \\ &= f + \mathcal{I} = \{f + h : h \in \mathcal{I}\}. \end{aligned}$$

The quotient of $k[x_1, \dots, x_n]$ modulo \mathcal{I} is the set of equivalence classes

$$k[x_1, \dots, x_n]/\mathcal{I} := \{[f] : f \in k[x_1, \dots, x_n]\}.$$

With addition $[f] + [g] := [f + g]$ and multiplication $[f] \cdot [g] := [f \cdot g]$ for all $f, g \in k[x_1, \dots, x_n]$, the quotient $k[x_1, \dots, x_n]/\mathcal{I}$ is a commutative ring.

2.2.6.2 Krull Dimension

The results on the Krull dimension presented in this subsection can be found in general literature about commutative algebra such as [41, 48, 71, 83].

An ideal \mathcal{I} in a ring R is called prime ideal if $p \in \mathcal{I}$ or $q \in \mathcal{I}$ for all $p, q \in R$ with $pq \in \mathcal{I}$.

Given a ring R , the Krull dimension $\dim_K R$ is the supremum of the lengths r of all chains of prime ideals $\mathcal{P}_0 \subset \mathcal{P}_1 \subset \dots \subset \mathcal{P}_r$ in R . It holds $\dim_K k[x_1, \dots, x_n] = n$.

Let $\mathcal{V} \subseteq k^n$ be an affine variety and \mathcal{I} an ideal in $k[x_1, \dots, x_n]$ such that $\mathcal{V} = \mathbf{V}(\mathcal{I})$. Then the dimension $\dim \mathcal{V}$ of \mathcal{V} is $\dim_K k[x_1, \dots, x_n]/\mathcal{I}$. This definition is independent of the choice of the ideal with $\mathcal{V} = \mathbf{V}(\mathcal{I})$.

The following lemma is proven in [41, Corollary 9.1].

Lemma 2.34. *Let \mathcal{I} be an ideal in $k[x_1, \dots, x_n]$. Then*

$$|\mathbf{V}(\mathcal{I})| < \infty \iff \dim \mathcal{V} = 0$$

is valid.

This is the reason why an ideal \mathcal{I} with $|\mathbf{V}(\mathcal{I})| < \infty$ is called zero-dimensional.

2.2.6.3 Formulation of the Shape Lemma

The Shape Lemma was first proven by Gianni et al. in [52, 53].

Lemma 2.35 (Shape Lemma). *Let k be a field and \mathcal{I} a zero-dimensional radical ideal in $k[x_1, \dots, x_n]$ such that all d complex roots of \mathcal{I} have distinct x_n -coordinates. Then the reduced Gröbner basis \mathcal{G} w.r.t. the lexicographic ordering of \mathcal{I} is of the shape*

$$\mathcal{G} = \{x_1 - q_1(x_n), x_2 - q_2(x_n), \dots, x_{n-1} - q_{n-1}(x_n), r(x_n)\}$$

where r is a polynomial of degree d and q_i is a polynomial of degree less than d for all $i = 1, \dots, n-1$.

It has already been pointed out that the computation of a Gröbner basis w.r.t. the lexicographic ordering reduces the problem of solving a system of multivariate polynomials to solving univariate polynomials. However, in the setting of the Shape Lemma 2.35, the reduced Gröbner basis w.r.t. the lexicographic ordering can do even better because the accumulated errors of the approximately determined solutions are smaller. In general, if the components of the solutions are determined in the order x_n, \dots, x_1 , then the approximation errors of the components x_n, \dots, x_{l-1} affect the component x_l so that the x_1 component depends on the approximation errors of all other components of the solution.

In contrast, if the conditions of the Shape Lemma 2.35 are met, then the components x_1, \dots, x_{n-1} depend only on the approximation error of component x_n , but x_1, \dots, x_{n-1} can be determined independently of each other.

2.3 Comprehensive Gröbner Systems

Another interesting task is to solve systems of polynomials containing some parameters. Here, comprehensive Gröbner systems play an important role. For an introduction on comprehensive Gröbner systems the reader is referred to [64, 87, 104].

In this section the polynomial ring $k[u_1, \dots, u_m][x_1, \dots, x_n]$, where x_1, \dots, x_n are indeterminates and u_1, \dots, u_m are parameters and $\{u_1, \dots, u_m\} \cap \{x_1, \dots, x_n\} = \emptyset$, is considered. A polynomial $f \in k[u_1, \dots, u_m][x_1, \dots, x_n]$ is a polynomial in x_1, \dots, x_n whose coefficients are polynomials in u_1, \dots, u_m . Let \bar{k} denote the algebraic closure of k . A specialization of $k[u_1, \dots, u_m]$ is a homomorphism

$$\sigma: k[u_1, \dots, u_m] \rightarrow \bar{k}.$$

For $a \in \bar{k}^m$ the specialization induced by a is defined

$$\sigma_a: k[u_1, \dots, u_m] \rightarrow \bar{k}, \quad g \mapsto g(a).$$

A specialization σ of $k[u_1, \dots, u_m]$ can be extended canonically to a specialization $\bar{\sigma}: k[u_1, \dots, u_m][x_1, \dots, x_n] \rightarrow \bar{k}[x_1, \dots, x_n]$ of $k[u_1, \dots, u_m][x_1, \dots, x_n]$ by applying σ coefficient-wise. In the following, both specializations will be denoted σ .

Definition 2.36 (Comprehensive Gröbner System). Let F be a set of polynomials in $k[u_1, \dots, u_m][x_1, \dots, x_n]$, $A_1, \dots, A_l \subseteq \bar{k}^m$ algebraically constructible sets such that $\bigcup_{i=1}^l A_i = \bar{k}^m$, and $\mathcal{G}_1, \dots, \mathcal{G}_l$ sets of polynomials in $k[u_1, \dots, u_m][x_1, \dots, x_n]$. The finite set $\tilde{\mathcal{G}} := \{(A_1, \mathcal{G}_1), \dots, (A_l, \mathcal{G}_l)\}$ is called a comprehensive Gröbner system for F if $\sigma_a(\mathcal{G}_i)$ is a Gröbner basis of the ideal $\langle \sigma_a(F) \rangle \subseteq \bar{k}[x_1, \dots, x_n]$ for all $a \in A_i$ and $i = 1, \dots, l$. Each pair (A_i, \mathcal{G}_i) is called a branch of $\tilde{\mathcal{G}}$.

In this thesis, the algebraically constructible sets A_i are of the form $A_i = \mathbf{V}(E_i) \setminus \mathbf{V}(N_i)$ with $E_i, N_i \subseteq k[u_1, \dots, u_m]$. A pair (E_i, N_i) is called a parametric constraint. For some further reading on constructible sets see, e.g., [6].

A comprehensive Gröbner system is called disjoint if the sets A_i are pairwise disjoint. It is called reduced if the sets $\sigma_a(\mathcal{G}_i)$ are reduced Gröbner bases of $\langle \sigma_a(F) \rangle \subseteq \bar{k}[x_1, \dots, x_n]$ for all $a \in A_i$ and $i = 1, \dots, l$.

Comprehensive Gröbner systems often suffer from a large number of branches what makes it hard to interpret them. The algorithms proposed in [87] and [64] focus on the computation of comprehensive Gröbner systems with as few branches as possible.

Chapter 3

Graph Theory

As will be seen later, gas networks can be modeled as (directed) graphs. This chapter deals with basic definitions and facts in graph theory. Complete introductions into graph theory can be found in [16, 17, 37, 38].

3.1 Graphs

3.1.1 Basic Definitions

A graph is a pair $G = (V, A)$ of two finite sets $V = V(G)$ and $A = A(G)$ such that $V \cap A = \emptyset$. The elements of V are called nodes, whereas the elements of A are referred to as edges. An edge $a \in A$ uniquely determines a set $\{u, v\}$ of nodes $u, v \in V$, written $a = \{u, v\}$. The nodes u and v are the end nodes of a . In a graph an edge whose end nodes coincide is called a loop. Two edges $a = \{u, v\}$ and $b = \{u, v\}$ are said to be parallel. A simple graph is one without loops and parallel edges.

Consider an edge $a = \{u, v\}$ in G . Then the edge a is incident to the nodes u and v , or a and u respectively a and v are incident. The nodes u and v are adjacent to each other and if $u \neq v$, they are called neighbors. The set of all neighbors of a node u is denoted $N_G(u)$. Given another edge $b = \{v, w\}$, the edges a and b are adjacent. For a node $u \in V$, the degree $\deg(u)$ is the number of edges incident to u .

A graph $G' = (V', A')$ is a subgraph of the graph $G = (V, A)$ if $V' \subseteq V$, $A' \subseteq A$ and each edge of G' has the same end nodes in G' as in G .

A walk is a finite alternating sequence of nodes and edges $u_1, a_1, u_2, a_2, \dots, a_{n-1}, u_n$ with $a_i = \{u_i, u_{i+1}\}$ and $a_i \neq a_j$ for all $i, j = 1, \dots, n-1$, $i \neq j$. A walk is called open if $u_1 \neq u_n$, otherwise it is closed. An open walk with $u_i \neq u_j$ for all $i, j = 1, \dots, n$, $i \neq j$, is a path. A cycle \mathcal{C} is a closed walk with $u_i \neq u_j$ for all $i, j = 1, \dots, n$, $i \neq j$, $i, j \neq 1, n$. Let C^+ denote the set of all cycles in G .

A graph G is connected if every pair of nodes in G is connected by a path in G . Otherwise, G is disconnected. A disconnected graph consists of several connected subgraphs called components.

A tree \mathcal{T} is a connected graph without any cycles. For a tree \mathcal{T} it holds $|A(\mathcal{T})| = |V(\mathcal{T})| - 1$. Furthermore, for two nodes $u, v \in V(\mathcal{T})$ there always is a path in \mathcal{T} connecting u and v . This path is uniquely determined and denoted $u\mathcal{T}v$. A tree \mathcal{T} is a spanning tree of a graph $G = (V, A)$ if \mathcal{T} is a subgraph of G and $V(\mathcal{T}) = V(G)$. It is easily seen that every connected graph contains at least one spanning tree. The subgraph $\overline{\mathcal{T}} = (V(G), A(G) \setminus A(\mathcal{T}))$ of G is the cotree of \mathcal{T} in G .

A fundamental cycle of a connected graph $G = (V, A)$ is a cycle arising by adding a non-tree edge $a \in A(\overline{\mathcal{T}})$ to a spanning tree \mathcal{T} of G . This uniquely determined cycle is denoted \mathcal{C}_a and the set of all fundamental cycles $C = C_{\mathcal{T}}$. On the contrary, for a fundamental cycle $\mathcal{C} \in C_{\mathcal{T}}$ let $a_{\mathcal{C}} \in A(\overline{\mathcal{T}})$ denote the edge not contained in the spanning tree that generates the fundamental cycle \mathcal{C} . For an edge $a \in A$ let C_a be the set of all fundamental cycles containing edge a . If C' is a subset of C , then $A_{C'}$ is the set of all arcs $a \in A$ that are arcs of the cycles in C' but not of those in $C \setminus C'$, i.e.,

$$A_{C'} := \{a \in A: a \in A(\mathcal{C}) \forall \mathcal{C} \in C', a \notin A(\mathcal{C}) \forall \mathcal{C} \in C \setminus C'\}.$$

It has to be mentioned that different spanning trees of a connected graph define different fundamental cycles, but the number of fundamental cycles stays the same, namely $|A| - |V| + 1$.

3.1.2 Depth First Search

The topic of this subsection is the construction of a spanning tree of a connected graph $G = (V, A)$. A tree-search is a method for this that starts with a subgraph G' of G that consists of exactly one arbitrary node in V . This node will be the root of the spanning tree constructed during the tree-search. In every step of this method an edge in A with its incident nodes is added to G' such that G' remains a tree. If no other edge with this property can be found, G' is a spanning tree of G since G is connected. There are several possible orders in which the edges can be added. The two most known algorithms using this method are breadth-first search and depth-first search. In this thesis spanning trees are always constructed via depth-first search (DFS), so this is the only algorithm discussed in this subsection.

Let \mathcal{T} be a spanning tree of G constructed with a tree-search algorithm, $r \in V$ the root of \mathcal{T} , and $u \in V$ a node. Every node in the unique path $r\mathcal{T}u$ connecting r and u in \mathcal{T} , including u , is an ancestor of u . An ancestor of u that is not u itself is a proper ancestor. Conversely, every node that u is an ancestor of is a descendant of u . The set of all descendants of u is denoted $D_{\mathcal{T}}(u)$. If $u \neq r$, the predecessor $p(u)$ of u is the immediate proper ancestor of u and the successor of u is the node whose predecessor is u .

The following algorithm can be found in [17].

Algorithm 3.1 (DFS-Algorithm).

Input: A connected graph $G = (V, A)$, a root $r \in V$

Output: A spanning tree \mathcal{T} of G with root r and a predecessor function p

```

 $S := (r)$ 
 $\mathcal{T} := (\{r\}, \emptyset)$ 
WHILE  $S \neq \emptyset$  DO
    consider the first node  $u$  in  $S$ 
    IF there exists  $a = \{u, v\} \in A(G)$  with  $v \notin V(\mathcal{T})$  DO
         $V(\mathcal{T}) := V(\mathcal{T}) \cup \{v\}$ 
         $p(v) := u$ 
         $A(\mathcal{T}) := A(\mathcal{T}) \cup \{a\}$ 
        add  $v$  to the top of  $S$ 
    ELSE DO
        remove  $u$  from  $S$ 
RETURN  $\mathcal{T}, p$ 

```

3.1.3 Matrix Representations

Graphs can be represented by node-edge incidence matrices, or incidence matrices for short. The node-edge incidence matrix of a graph $G = (V, A)$ is a $|V| \times |A|$ matrix \mathcal{A}^+ over \mathbb{R} defined

$$a_{i,j} := \begin{cases} 1 & \text{if edge } a_j \text{ is incident to node } u_i, \\ 0 & \text{otherwise.} \end{cases}$$

The following three propositions are proven in [37].

Proposition 3.2. *If a graph $G = (V, A)$ consists of k components, then $\text{rank}(\mathcal{A}^+) = |V| - k$.*

This means that, if G is connected, an arbitrary row can be deleted from \mathcal{A}^+ without information getting lost. This yields a $(|V| - 1) \times |A|$ submatrix \mathcal{A} of \mathcal{A}^+ , called reduced incidence matrix. Then the reference node is the node corresponding to the row deleted.

Proposition 3.3. *Let $G = (V, A)$ be a connected graph and \mathcal{A} a reduced incidence matrix of G . A $(|V| - 1) \times (|V| - 1)$ submatrix of \mathcal{A} is nonsingular if and only if there is a spanning tree of G whose edges are exactly the $|V| - 1$ edges corresponding to the columns of this submatrix.*

Corollary 3.4. *Every reduced incidence matrix of a tree is nonsingular.*

For a given connected graph G and a spanning tree \mathcal{T} of G this motivates the representation

$$\mathcal{A} = [\mathcal{A}_B \mid \mathcal{A}_N]$$

where the columns of the $(|V| - 1) \times (|V| - 1)$ matrix \mathcal{A}_B correspond to the edges of the spanning tree \mathcal{T} and thus \mathcal{A}_B is nonsingular.

The $|A| \times (|A| - |V| + 1)$ matrix $\mathcal{B} = \mathcal{B}_{\mathcal{T}}$ representing the fundamental cycles of a connected graph $G = (V, A)$ with respect to the spanning tree \mathcal{T} is defined

$$b_{i,j} := \begin{cases} 1 & \text{if fundamental cycle } \mathcal{C}_j \text{ contains edge } a_i, \\ 0 & \text{otherwise} \end{cases}$$

and rearranging the rows yields

$$\mathcal{B} = \begin{bmatrix} \mathcal{B}_B \\ \mathcal{B}_N \end{bmatrix} = \begin{bmatrix} \mathcal{B}_B \\ I_{|A|-|V|+1} \end{bmatrix}$$

where the last $|A| - |V| + 1$ rows correspond to the edges that are not contained in the spanning tree \mathcal{T} of G . This implies $\text{rank}(\mathcal{B}) = |A| - |V| + 1$.

Proposition 3.5. *Let $G = (V, A)$ be a connected graph with spanning tree \mathcal{T} , reduced incidence matrix \mathcal{A} and fundamental cycle matrix \mathcal{B} . Then*

$$\mathcal{A}_B^{-1} \mathcal{A}_N = \mathcal{B}_B \pmod{2}.$$

3.2 Digraphs

A directed graph or digraph is a graph with directions assigned to the edges. More formally, a digraph is a pair $G = (V, A)$ of two finite sets V and A such that $V \cap A = \emptyset$. Again, the elements of V are called nodes, but the directed elements of A are referred to as arcs. An arc $a \in A$ uniquely determines an ordered tuple (u, v) of nodes $u, v \in V$, written $a = (u, v)$. The nodes u and v are the end nodes of a . More precisely, u is the tail and v the head of a , denoted $\text{head}(a)$ and $\text{tail}(a)$, respectively, and a goes from u to v .

A digraph is an orientation of a graph G if it is obtained from G by assigning directions to the edges of G . An orientation of G is denoted \vec{G} .

Some of the definitions made for graphs can be adopted to digraphs, others need slight modifications. In this section only the definitions and statements that need to be modified are mentioned.

In addition to the degree, each node $u \in V$ has an in-degree of ingoing arcs and an out-degree of outgoing arcs, i.e., $\text{deg}^{\text{in}}(u) := |\{a : a = (v, u) \in A\}|$ and $\text{deg}^{\text{out}}(u) := |\{a : a = (u, v) \in A\}|$.

Defining walks, paths and cycles one has to distinguish between directed and undirected walks, paths, and cycles. A walk is a finite alternating sequence of nodes and arcs $u_1, a_1, u_2, a_2, \dots, a_{n-1}, u_n$ with $a_i = (u_i, u_{i+1})$ or $a_i = (u_{i+1}, u_i)$ and $a_i \neq a_j$ for all $i, j = 1, \dots, n-1$, $i \neq j$. It is directed if $a_i = (u_i, u_{i+1})$ holds for every $i = 1, \dots, n-1$. (Directed) paths and (directed) cycles in digraphs are defined equivalently.

The term connectivity splits up into strong and weak connectivity. A digraph is weakly connected, or simply connected, if every pair of nodes in it is connected by a not necessarily directed path and strongly connected if every pair of nodes is connected by a directed path. The definition of component stays the same, so that the components of a digraph can be weakly or strongly connected.

An r -branching is a rooted tree \mathcal{T} with $\deg^{\text{in}}(r) = 0$ and $\deg^{\text{in}}(u) = 1$ for all $u \in V(\mathcal{T})$ with $u \neq r$. In an r -branching \mathcal{T} , for every node $u \in V(\mathcal{T})$ there is a uniquely determined directed path from r to u .

The node-arc incidence matrix of a digraph $G = (V, A)$ is a $|V| \times |A|$ matrix \mathcal{A}^+ (over \mathbb{R}) defined

$$a_{i,j} := \begin{cases} 1 & \text{if node } u_i \text{ is head of arc } a_j, \\ -1 & \text{if node } u_i \text{ is tail of arc } a_j, \\ 0 & \text{otherwise.} \end{cases}$$

The fundamental cycles of a connected digraph $G = (V, A)$ with respect to the spanning tree \mathcal{T} are represented by the $|A| \times (|A| - |V| + 1)$ matrix $\mathcal{B} = \mathcal{B}_{\mathcal{T}}$ defined

$$b_{i,j} := \begin{cases} 1 & \text{if fundamental cycle } \mathcal{C}_j = \mathcal{C}_a \text{ contains arc } a_i, \text{ and } a_i \text{ and } a \text{ have the} \\ & \text{same direction in the cycle,} \\ -1 & \text{if fundamental cycle } \mathcal{C}_j = \mathcal{C}_a \text{ contains arc } a_i, \text{ and } a_i \text{ and } a \text{ have} \\ & \text{opposite directions in the cycle,} \\ 0 & \text{otherwise.} \end{cases}$$

All the propositions made about (reduced) incidence matrices and (reduced) cycle matrices of graphs can be adopted to the corresponding matrices of digraphs. Only Proposition 3.5 needs to be modified.

Proposition 3.6. *Let $G = (V, A)$ be a connected digraph with spanning tree \mathcal{T} , reduced incidence matrix \mathcal{A} and fundamental cycle matrix \mathcal{B} . Then*

$$\mathcal{A}_B^{-1} \mathcal{A}_N = -\mathcal{B}_B.$$

In addition to the above properties of and the relations between the matrices representing a digraph, the meaning of the inverse of the basis part of the reduced incidence matrix \mathcal{A}_B^{-1} is needed.

Consider a connected digraph $G = (V, A)$ with spanning tree \mathcal{T} rooted in $r \in V$. The unique paths in \mathcal{T} connecting each node to the root r are represented in the $(|V| - 1) \times (|V| - 1)$ matrix $\mathcal{P} = \mathcal{P}_{\mathcal{T}}$ defined

$$p_{i,j} := \begin{cases} 1 & \text{if the path } r\mathcal{T}u_j \text{ contains arc } a_i \text{ and } a_i \text{ is directed towards } u_j, \\ -1 & \text{if the path } r\mathcal{T}u_j \text{ contains arc } a_i \text{ and } a_i \text{ is directed towards } r, \\ 0 & \text{otherwise.} \end{cases}$$

If \mathcal{P} is the path matrix of an r -branching, then all entries of \mathcal{P} are either 0 or 1.

Proposition 3.7. *Let $G = (V, A)$ be a connected digraph with spanning tree \mathcal{T} . Then*

$$\mathcal{A}_B^{-1} = \mathcal{P}.$$

Proof. It suffices to show that \mathcal{P} is a right inverse of \mathcal{A}_B , i.e., $\mathcal{A}_B \mathcal{P} = I_{|V|-1}$. For each $i, j = 1, \dots, |V| - 1$ consider the product of the i -th row of \mathcal{A}_B and the j -th column of \mathcal{P}

$$(\mathcal{A}_B)_{i,\bullet} \mathcal{P}_{\bullet,j} = \sum_{k=1}^{|V|-1} a_{i,k} p_{k,j}.$$

The entry $a_{i,k}$ is nonzero if and only if arc a_k is incident to node u_i .

If $i = j$, then exactly one arc incident to u_i is in the path connecting r and u_i . Thus there is exactly one $k \in \{1, \dots, |V| - 1\}$ where both $(\mathcal{A}_B)_{i,\bullet}$ and $\mathcal{P}_{\bullet,j}$ have nonzero entries. If u_i is the head of a_k , then a_k is directed towards u_i and $(\mathcal{A}_B)_{i,\bullet} \mathcal{P}_{\bullet,j} = 1 \cdot 1 = 1$. If u_i is the tail of a_k , then a_k is directed towards r and $(\mathcal{A}_B)_{i,\bullet} \mathcal{P}_{\bullet,j} = -1 \cdot (-1) = 1$.

Now let $i \neq j$. If node u_i does not lie in the path p connecting the root r and u_j , then none of the arcs incident to u_i can be contained in the path p and hence $a_{i,k} p_{k,j} = 0$ for all $k = 1, \dots, |V| - 1$. If node u_i is contained in path p , then exactly two arcs incident to u_i are in p . If u_i is the tail of one of these arcs and head of the other, i.d., the two arcs are directed in the same direction, then $(\mathcal{A}_B)_{i,\bullet} \mathcal{P}_{\bullet,j} = -1 \cdot 1 + 1 \cdot 1 = 0$ or $(\mathcal{A}_B)_{i,\bullet} \mathcal{P}_{\bullet,j} = -1 \cdot (-1) + 1 \cdot (-1) = 0$. If u_i is the tail of both of these arcs or the head of both of these arcs, i.d., the two arcs are directed in opposite direction, then $(\mathcal{A}_B)_{i,\bullet} \mathcal{P}_{\bullet,j} = 1 \cdot 1 + 1 \cdot (-1) = 0$ or $(\mathcal{A}_B)_{i,\bullet} \mathcal{P}_{\bullet,j} = -1 \cdot 1 + -1 \cdot (-1) = 0$. \square

Chapter 4

Modeling Gas Networks

This chapter deals with the modeling of gas networks. In Section 4.1 physical properties of gas are listed and in Section 4.2 these properties are used to model gas flow along single pipes via the Euler equations. General introductions into modeling of gas flow are given in [68, 77, 84] and many other books. Furthermore, in Section 4.2 the model of a single pipe is reformulated in an algebraic model.

As it is a common practice, gas networks are modeled as graphs in Section 4.3.

4.1 Physical Properties of Gas

In this thesis, some assumptions about the network and the gas flow are needed. The gas flow is considered to be one-dimensional. This means that pressure, density, and velocity depend only on the time and the location along the axis of the pipe, but not on the location in the cross section. For this it is required that these physical quantities can be approximated good enough by their mean values over the cross section. If, in addition to that, the pipes of the network are cylindrical and the cross sections are constant along the pipe, the relation between the mass flow q in kg s^{-1} , density ρ in kg m^{-3} and the velocity v in m s^{-1} can be described by

$$q = A\rho v, \quad (4.1)$$

where A is the cross-sectional area in m^2 .

In the literature, mostly the mass flow q in kg s^{-1} is used, whereas throughout this thesis the volumetric flow rate under normal conditions Q_0 in $\text{m}^3 \text{h}^{-1}$ is considered, which can be converted via the equation

$$q = \frac{1}{60^2} \rho_0 Q_0, \quad (4.2)$$

where ρ_0 denotes the density of the gas under normal conditions in kg m^{-3} . The normal conditions are specified in DIN 1343 [39]. The norm temperature is $T_0 = 273.15 \text{ K}$ and the norm pressure is $p_0 = 101325 \text{ Pa}$.

Moreover, pipes are presumed to be horizontal and the network contains only one gas mixture.

The model considered in this thesis is isothermal and stationary. The former states that gas and surrounding soil have a constant temperature, the latter implies that there are no changes over time and that all injections and withdrawals of gas occur at a fixed rate. Then the steady state of the network is the state in which the network would be after an arbitrarily long time without changes from the outside.

4.1.1 Equation of State for Real Gases

The equation of state for ideal gases connects the density ρ , pressure p in Pa, molar mass m in kg mol^{-1} and temperature T in K of a gas and reads

$$p = \rho R_s T,$$

where $R_s = \frac{R}{m}$ is the specific gas constant of the gas in $\text{J kg}^{-1} \text{K}^{-1}$ with universal gas constant $R = 8.31441 \text{ J mol}^{-1} \text{K}^{-1}$.

Real gases do not behave the same way as ideal gases do because in real gases the molecules interact with each other. Therefore, the equation of state for ideal gases has to be corrected by a factor z called real gas factor or compressibility factor. This yields the thermodynamical standard equation of state for real gases

$$p = \rho R_s T z. \quad (4.3)$$

More detailed discussions of the equation of state of ideal and real gases can be found in [77, 84] and others.

4.1.1.1 Compressibility Factor

For a given temperature and pressure the compressibility factor of a gas is the ratio of the gas volume to the gas volume the gas would have if it were an ideal gas at the same temperature. Thus, it depends on its pressure and temperature as well as on its chemical composition. For ideal gases the compressibility factor equals 1.

The compressibility factor cannot be given exactly, but for pressures up to 7000000 Pa a formula from the American Gas Association (AGA) turns out to be accurate ([69]):

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

The quantity T_c denotes the pseudocritical temperature of the gas in K and p_c the pseudocritical pressure in Pa, see [84]. The meaning of these two quantities is the following: The critical temperature of a pure gas is the temperature above which the gas cannot be liquefied under pressure. The critical pressure of a pure gas is the minimum pressure needed to liquefy a gas at its critical temperature. For gas mixtures critical temperature and critical pressure are called pseudocritical.

For the computation of z the mean pressure

$$p_m = \frac{1}{2} (\max \{ \underline{p}_{\text{in}}, \underline{p}_{\text{out}} \} + \min \{ \bar{p}_{\text{in}}, \bar{p}_{\text{out}} \})$$

along the pipe is used, where $\underline{p}_{\text{in}}$ and \bar{p}_{in} are the lower respectively upper pressure bounds at the beginning of the pipe and $\underline{p}_{\text{out}}$ and \bar{p}_{out} are the lower respectively upper pressure bounds at the end of the pipe. This gives rise to the definition $z_m := z(p_m, T)$.

The compressibility factor under normal conditions, $z(p_0, T_0)$, is denoted z_0 .

4.1.2 Friction Factor

The roughness of the wall of the inner side of the pipe, the curvature of the pipe, corrosion processes, and the deposition of dirt and dust in the pipe, summarized under the term integral roughness k in m, cause friction. This friction implies a pressure drop of the gas flowing through the pipe.

To determine the friction factor $\lambda = \lambda(Q_0)$ the Reynolds number (see, e.g., [68, 77, 84])

$$\text{Re} = \text{Re}(Q_0) = \frac{4 \rho_0}{60^2 \pi \eta D} Q_0,$$

where η in Pa s is the dynamic viscosity of the gas, is needed. For natural gas it is about 10^{-5} Pa s. The Reynolds number indicates if the gas flow is laminar or turbulent. If $\text{Re} \geq \text{Re}_{\text{crit}} = 2320$, the flow is turbulent, i.e., vortex flow with mixing layers. Otherwise it is laminar, which means that the flow is layerwise.

For laminar flow a common formula for the friction factor is the Stokes formula

$$\lambda = \frac{64}{\text{Re}},$$

see, e.g., [77].

Due to [84], in the turbulent case the equation of Coolebrook-White

$$\frac{1}{\sqrt{\lambda}} = -2 \log_{10} \left(\frac{2.51}{\text{Re} \sqrt{\lambda}} + \frac{k}{3.71 D} \right)$$

can be used. The explicit formula

$$\lambda = \left(2 \log_{10} \left(\frac{4.518}{\text{Re}} \log_{10} \left(\frac{\text{Re}}{7} + \frac{k}{3.71 D} \right) \right) \right)^{-2}$$

is given by Hofer ([68]).

4.2 Single Pipes

4.2.1 Euler Equations

The gas flow along a single pipe can be modeled via the Euler Equations (for a deduction of the equations see, e.g., [12, 77])

$$A \frac{\partial \rho}{\partial t} + \frac{\partial q}{\partial x} = 0 \quad (4.4)$$

$$\frac{\partial p}{\partial x} + \lambda \frac{|v|v}{2D} \rho + \frac{1}{A} \frac{\partial q}{\partial t} + g\rho s + \frac{1}{A} \frac{\partial \rho v^2}{\partial x} = 0 \quad (4.5)$$

where t is the time in s, $x \in [0, L]$ the location in the pipe in m, $s \in [-1, 1]$ the slope of the pipe and $g = 9.80665 \text{ m s}^{-2}$ the gravitational acceleration. Equation (4.4) is called continuity equation and models the conservation of mass. The momentum equation (4.5) represents the conservation of momentum. It describes how the pressure drop along the pipe depends on the mass flow and some technical parameters summarized in λ . Since in this thesis only the isothermal case is considered, the energy equation is neglected here.

Equations (4.4) and (4.5) build a system of two nonlinear, hyperbolic, partial differential equations in four indeterminates q , p , ρ , and v . The system is completed by equations (4.1) and (4.3). Then the entire system reads

$$A \frac{\partial \rho}{\partial t} + \frac{\partial q}{\partial x} = 0 \quad (4.4 \text{ revisited})$$

$$\frac{\partial p}{\partial x} + \lambda \frac{|v|v}{2D} \rho + \frac{1}{A} \frac{\partial q}{\partial t} + g\rho s + \frac{1}{A} \frac{\partial \rho v^2}{\partial x} = 0 \quad (4.5 \text{ revisited})$$

$$A\rho v = q \quad (4.1 \text{ revisited})$$

$$\rho R_s T z = p. \quad (4.3 \text{ revisited})$$

4.2.2 Algebraic Model

This system can be transformed into a single algebraic equation. Similar reformulations can be found in, e.g., [12, 68, 100].

Since only the stationary case is considered in this thesis, the derivatives w.r.t. the time t are zero. Continuity equation (4.4) thus becomes

$$\frac{\partial q}{\partial x} = 0$$

and hence the mass flow q is constant along the pipe. Relation (4.2) then yields that the volumetric flow rate under normal conditions Q_0 is constant along the pipe as well.

In momentum equation (4.5), the term $\frac{1}{A} \frac{\partial q}{\partial t}$ is zero for the same reason as above. Moreover, $g\rho s = 0$ because pipes are assumed to be horizontal. Due to

[105], the term $\frac{1}{A} \frac{\partial \rho v^2}{\partial x}$ makes a contribution of less than one percent to the sum under normal operating conditions and hence can be neglected. This implies

$$\frac{\partial p}{\partial x} = -\lambda \frac{|v|v}{2D} \rho. \quad (4.6)$$

Inserting equations (4.1) and (4.2) together with $A = \frac{\pi D^2}{4}$ into (4.6) yields

$$\frac{\partial p}{\partial x} = -\lambda(Q_0) \frac{16 \rho_0^2 |Q_0| Q_0}{60^2 60^2 \pi^2 2 D^5 \rho}. \quad (4.7)$$

Since equation (4.3) also holds under normal conditions,

$$\frac{\rho_0}{\rho} = \frac{p_0 T z_m}{p T_0 z_0}$$

is valid. Inserting this equation into equation (4.7) leads to

$$\frac{\partial p}{\partial x} = -\lambda(Q_0) \frac{16 \rho_0 p_0 T z_m}{60^2 60^2 \pi^2 2 D^5 p T_0 z_0} |Q_0| Q_0,$$

which is equivalent to

$$2p \frac{\partial p}{\partial x} = -\lambda(Q_0) \frac{16 \rho_0 p_0 T z_m}{60^2 60^2 \pi^2 D^5 T_0 z_0} |Q_0| Q_0. \quad (4.8)$$

Integration of (4.8) w.r.t. the location x implies

$$\begin{aligned} \int_0^L 2p \frac{\partial p}{\partial x} dx &= \int_0^L -\lambda(Q_0) \frac{16 \rho_0 p_0 T z_m}{60^2 60^2 \pi^2 D^5 T_0 z_0} |Q_0| Q_0 dx \\ \Leftrightarrow \int_{p(0)}^{p(L)} 2u du &= -\lambda(Q_0) \frac{16 \rho_0 p_0 T z_m}{60^2 60^2 \pi^2 D^5 T_0 z_0} |Q_0| Q_0 \int_0^L 1 dx \\ \Leftrightarrow [u^2]_{p_{\text{in}}}^{p_{\text{out}}} &= -\lambda(Q_0) \frac{16 \rho_0 p_0 T z_m}{60^2 60^2 \pi^2 D^5 T_0 z_0} |Q_0| Q_0 [x]_0^L \\ \Leftrightarrow p_{\text{out}}^2 - p_{\text{in}}^2 &= -\lambda(Q_0) \underbrace{\frac{16 \rho_0 p_0 T z_m L}{60^2 60^2 \pi^2 D^5 T_0 z_0}}_{=: \phi} |Q_0| Q_0 \end{aligned} \quad (4.9)$$

The coefficient ϕ is called pressure drop coefficient. The pressure drop is the reduction of fluid-mechanical energy.

4.3 Networks

4.3.1 Conservation of Mass at the Junctions

A gas network consists of several pipes that are connected at junctions. At a junction of several pipes the mass of the gas remains constant. Let I denote the

set of pipes through which gas flows towards the junction and J the set of pipes through which gas flows away from the junction. Then

$$\sum_{i \in I} Q_{0,i} = \sum_{j \in J} Q_{0,j}. \quad (4.10)$$

4.3.2 Modeling Gas Networks Using Graphs

Gas networks can be modeled as connected graphs $G = (V^+, A)$ where the set of nodes V^+ consists of the junctions of the network and the edges in A correspond to the pipes of the network. The set of the nodes V^+ is the union of the three disjoint sets V_+ of the entry nodes where gas is injected into the network, V_- of the exit nodes where gas is withdrawn from the network and V_0 of nodes that are neither entries nor exits, referred to as innodes.

Using DFS-Algorithm 3.1 described in Subsection 3.1.2 with root $r \in V_+$ a spanning tree of G can be computed. The edge set of this spanning tree can be oriented by its predecessor function p yielding the oriented tree \mathcal{T} with arcs

$$A(\mathcal{T}) := \{(p(u), u) : u \in V(\mathcal{T}) \setminus \{r\}\}.$$

Orienting the edges in $\overline{\mathcal{T}}$ in such a way that no directed cycles occur, an orientation \vec{G} of G is obtained. The oriented tree \mathcal{T} is a spanning tree of \vec{G} rooted in r . Since every node has exactly one predecessor, \mathcal{T} is an r -branching.

Let \mathcal{A}^+ denote the incidence matrix of \vec{G} . By Proposition 3.2, an arbitrary row of \mathcal{A}^+ can be deleted. For this purpose the root r is chosen as the reference node and from now on it will always be indexed with 0. The resulting reduced incidence matrix is denoted \mathcal{A} and $V := V^+ \setminus \{r\}$. Let the rows of \mathcal{A} be arranged such that

$$\mathcal{A} = [\mathcal{A}_B \mid \mathcal{A}_N]$$

where the columns of the $|V| \times |V|$ matrix \mathcal{A}_B correspond to the arcs of the spanning tree \mathcal{T} . Due to Corollary 3.4, \mathcal{A}_B is nonsingular and hence \mathcal{A}_B^{-1} exists.

Let $Q_0 \in \mathbb{R}^{|A|}$ be the vector containing for each arc $a \in A$ of \vec{G} the volumetric flow rate under normal conditions $Q_{0,a}$. Then for $Q_{0,a} > 0$ the gas flows from the tail of arc a to the head of arc a and vice versa for $Q_{0,a} < 0$. Thus, one has to distinguish between two different orientations of the arcs: the orientation w.r.t. the spanning tree \mathcal{T} computed with the DFS-Algorithm 3.1 and the orientation corresponding to the flow direction of the gas. To make clear which direction is meant in the rest of the thesis all quantities related to arc orientation, for example the degree of a node, are indexed by the subscripts ‘‘DFS’’ respectively ‘‘gas’’. For instance, $\deg_{\text{DFS}}^{\text{in}}(u)$ denotes the indegree of node u w.r.t. the spanning tree \mathcal{T} , whereas $\deg_{\text{gas}}^{\text{in}}(u)$ denotes the indegree of node u w.r.t. the flow direction of the gas.

Furthermore, let $p^+, q^{\text{nom}+} \in \mathbb{R}^{|V^+|}$ denote the vectors containing for each node $u \in V^+$ the pressure p_u and load q_u^{nom} , respectively, and $\Phi = \text{diag}(\phi_{a_1}, \dots, \phi_{a_{|A|}}) \in$

$\mathbb{R}^{|A| \times |A|}$ a matrix whose nonzero entry ϕ_{a_i} is the pressure drop coefficient of arc a_i introduced at the end of the previous section for $i = 1, \dots, |A|$. Pressures at nodes are limited by lower and upper bounds. Upper bounds stem from physical limitations of the network, while lower bounds depend on the contracts with costumers. Lower and upper pressure bounds are both strictly positive. The vector of the lower bounds \underline{p}_u is denoted \underline{p}^+ and the vector of the upper bounds \bar{p}_u is denoted \bar{p}^+ . A load q_u^{nom} is nonnegative if u is an exit node, nonpositive if u is an entry node and zero if u is an innode. Because an entry node or an exit node with zero load can be treated as an innode, the loads of entry nodes and exit nodes are assumed to be nonzero. Since conservation of mass holds at every junction (see Subsection 4.3.1), the same amount of gas has to be withdrawn from the network that is injected into it. This leads to the necessity of balanced load vectors, i.e., $\mathbb{1}^T q^{\text{nom}+} = 0$.

The symbols $+$, $-$, 0 as subscripts of vectors in $\mathbb{R}^{|V^+|}$ are used to extract the components indexed by elements in V_+ , V_- , and V_0 , respectively. For instance, $q_-^{\text{nom}} = (q_u^{\text{nom}})_{u \in V_-}$. The load q_0^{nom} at the innodes V_0 is zero. The subscripts B and N of vectors in $\mathbb{R}^{|A|}$ are used to extract the components indexed by arcs in \mathcal{T} and $\bar{\mathcal{T}}$, respectively. When used as subscripts of matrices whose columns are indexed by the elements of A , the subscripts extract the columns indexed by the arcs in \mathcal{T} and $\bar{\mathcal{T}}$, respectively. Moreover, for vectors whose entries correspond to nodes the superscript $+$ is used to indicate the full vector with entries indexed by elements in V^+ . Without the superscript $+$, entries of those vectors are indexed by the elements in V only.

With this notation, equation (4.10) for the conservation of mass at node $u \in V^+$ is equivalent to

$$\left(\mathcal{A}^+\right)_{u,\bullet} Q_0 = q_u^{\text{nom}+}.$$

Since this equation holds for every node $u \in V^+$,

$$\mathcal{A}^+ Q_0 = q^{\text{nom}+}$$

is valid. As observed above, \mathcal{A}^+ has rank n and $\mathbb{1}^T q^{\text{nom}+} = 0$, and thus, above system has the same solution space as

$$\mathcal{A} Q_0 = q^{\text{nom}}. \quad (4.11)$$

For a vector $v \in \mathbb{R}^s$ set $v^2 := (v_1^2, \dots, v_s^2)^T$ and $|v|v := (|v_1|v_1, \dots, |v_s|v_s)^T$. Then for arc $a \in A$, equation (4.9) can be reformulated as

$$\left(\mathcal{A}^+\right)_{\bullet,a}^T \left(p^+\right)^2 = -\phi_a |Q_{0,a}| Q_{0,a}$$

and thus the entire network has to satisfy

$$\mathcal{A}^{+T} \left(p^+\right)^2 = -\Phi |Q_0| Q_0. \quad (4.12)$$

System (4.11), (4.12) consists of $|V| + |A|$ equations, namely $|V|$ equations for the conservation of mass at the nodes in (4.11) and $|A|$ equations for the pressure drop along the pipes in (4.12), but contains $|V^+| + |A|$ indeterminates, namely $|A|$ indeterminates for the flows along the pipes and $|V^+|$ indeterminates for the pressures at the nodes. Thus fixing the pressure at the reference node, the flow along the pipes and the pressure at the remaining nodes become computable.

As shown, e.g., in [57, 100], equation (4.12) is equivalent to

$$\begin{aligned} \left(\mathcal{A}_{r,\bullet}^+\right)_B^T p_r^2 + \mathcal{A}_B^T p^2 &= -\Phi_B |Q_{0,B}| Q_{0,B} \\ \left(\mathcal{A}_{r,\bullet}^+\right)_N^T p_r^2 + \mathcal{A}_N^T p^2 &= -\Phi_N |Q_{0,N}| Q_{0,N}. \end{aligned}$$

Since the rows of a node-arc incidence matrix sum up to zero, $\left(\mathcal{A}_{r,\bullet}^+\right)_B = -\mathbf{1}^T \mathcal{A}_B$ holds and by multiplying the first equation by $\left(\mathcal{A}_B^{-1}\right)^T$ one gets

$$p^2 = \mathbf{1} p_r^2 - \mathcal{A}_B^{-1T} \Phi_B |Q_{0,B}| Q_{0,B}. \quad (4.13)$$

Part II

Problems related to Gas Networks

Chapter 5

Feasibility of Loads

In this chapter feasible load vectors are characterized. Moreover, two methods to reduce the effort that has to be made to solve the system of equations and inequalities are discussed: the fixation of the flow direction and redundant pressure bounds. For special networks an upper bound for the number of feasible flow directions is given.

5.1 The Set of Feasible Load Vectors

Summarizing the results of the previous chapter, for a given network the set of feasible load vectors is defined

$$M := \left\{ q^{\text{nom}+} : \mathbf{1}^T q^{\text{nom}+} = 0 \text{ and } \exists (Q_0, p^+) \in \mathbb{R}^{|A|+|V^+|} \text{ with } p^+ \in [\underline{p}^+, \bar{p}^+] \right. \\ \left. \text{fulfilling (4.11) and (4.12)} \right\}.$$

The following theorem in [57] gives a characterization of the set of feasible load vectors that reduces the number of equations and indeterminates.

Theorem 5.1. *Let G be a graph representing a given network, \mathcal{T} a DFS-tree rooted in the reference node r oriented w.r.t. the predecessor function, and \vec{G} the orientation of G w.r.t. the spanning tree \mathcal{T} . Define the map*

$$g: \mathbb{R}^{|V|} \times \mathbb{R}^{|A(\vec{\mathcal{T}})|} \rightarrow \mathbb{R}^{|V|}, \quad (s, t) \mapsto \left(\mathcal{A}_B^{-1} \right)^T \Phi_B \left| \mathcal{A}_B^{-1}(s - \mathcal{A}_{Nt}) \right| \left(\mathcal{A}_B^{-1}(s - \mathcal{A}_{Nt}) \right).$$

Then the set M consists of all $q^{\text{nom}+}$ with $\mathbf{1}^T q^{\text{nom}+} = 0$ for which there is a z such that

$$\mathcal{A}_N^T g(q^{\text{nom}}, z) = \Phi_N |z| z \tag{5.1}$$

$$\min_{i=1, \dots, |V|} \left[(\bar{p}_{u_i})^2 + g_i(q^{\text{nom}}, z) \right] \geq \max_{i=1, \dots, |V|} \left[(\underline{p}_{u_i})^2 + g_i(q^{\text{nom}}, z) \right] \tag{5.2}$$

$$(\underline{p}_r)^2 \leq \min_{i=1, \dots, |V|} \left[(\bar{p}_{u_i})^2 + g_i(q^{\text{nom}}, z) \right] \tag{5.3}$$

$$(\bar{p}_r)^2 \geq \max_{i=1, \dots, |V|} \left[(\underline{p}_{u_i})^2 + g_i(q^{\text{nom}}, z) \right]. \tag{5.4}$$

Similar reformulations and variable reductions of this problem can be found in [19, 20, 24]. System (5.1) has $|A(\overline{\mathcal{T}})|$ equations and $|A(\overline{\mathcal{T}})|$ indeterminates.

For a given load vector $q^{\text{nom}+}$ let $\hat{z}(q^{\text{nom}})$ be a solution of system (5.1). Then the corresponding flow $Q_0(q^{\text{nom}})$ can be determined from $\hat{z}(q^{\text{nom}})$ in the following way:

$$\begin{aligned} Q_{0,N}(q^{\text{nom}}) &= \hat{z}(q^{\text{nom}}) \\ Q_{0,B}(q^{\text{nom}}) &= \mathcal{A}_B^{-1} q^{\text{nom}} - \mathcal{A}_B^{-1} \mathcal{A}_N \hat{z}(q^{\text{nom}}). \end{aligned}$$

If $q^{\text{nom}+}$ is not feasible, then the intersection

$$\begin{aligned} F &= \left[\max_{i=1,\dots,|V|} \left[(\underline{p}_{u_i})^2 + g_i(q^{\text{nom}}, \hat{z}(q^{\text{nom}})) \right], \min_{i=1,\dots,|V|} \left[(\overline{p}_{u_i})^2 + g_i(q^{\text{nom}}, \hat{z}(q^{\text{nom}})) \right] \right] \\ &\cap \left[\underline{p}_r^2, \overline{p}_r^2 \right] \end{aligned}$$

is empty by Theorem 5.1. Otherwise, F is nonempty and in the proof of Theorem 5.1 in [57] it is shown that the pressure square p_r^2 can be chosen in F . By equation (4.13) and the definition of g the resulting pressures at the remaining nodes are

$$p_{u_i} = \sqrt{p_r^2 - g_i(q^{\text{nom}}, \hat{z}(q^{\text{nom}}))} \quad (5.5)$$

for $i = 1, \dots, |V|$.

Let $q^{\text{nom}} \in \mathbb{R}^{|V|}$ be an arbitrary reduced load vector and let $\mathcal{F}: \mathbb{R}^{|A(\overline{\mathcal{T}})|} \rightarrow |A(\overline{\mathcal{T}})|$ be defined

$$z \mapsto \Phi_N |z| z - \mathcal{A}_N^T g(q^{\text{nom}}, z).$$

The crucial fact is that

$$\mathcal{F}(z) = 0 \quad (5.6)$$

has a uniquely determined real solution. This means that for a given load vector the flow along the pipes is uniquely determined. Proofs can be found in [100] where coercive operators are used to prove the existence of a solution, and [19, 20] where strictly monotone basins on Hilbert spaces are utilized. In [103] the existence is proven via the Hartman-Stampacchia fixed point theorem ([60]). Uniqueness of the solution is verified in all of these works.

If the absolute values in \mathcal{F} are resolved, system (5.6) becomes a multivariate polynomial system. Thus, for each possible resolving of the absolute values system (5.6) can be solved with the Gröbner basis method of Subsection 2.2.5. Afterwards, it has to be checked if these solutions fulfill the conditions for the resolving of the absolute values. Since the original system (5.6) has a uniquely determined real solution, these conditions hold for exactly one of those solutions. Moreover, there can occur some systems that do not have any solution. If the reduced Gröbner basis contains the constant polynomial 1, the system does not have any solution and thus, it does not have to be solved. On the contrary, by the Weak Nullstellensatz 2.2 the reduced Gröbner basis of every system without solution contains the constant polynomial 1. Hence, the procedure does not try to solve systems that do not have any solution.

The procedure is summarized in the following algorithm. The first FOR-loop of the algorithm iterates over all possible combinations of resolvings of the absolute values.

Algorithm 5.2 (Check for Feasibility of Load Vector).

Input: Matrices \mathcal{A}^+ and Φ and vectors \underline{p}^+ and \bar{p}^+ representing the network,
a reference node r , a load vector $q^{\text{nom}+}$

Output: True, if $q^{\text{nom}+} \in M$, and False otherwise

```

FOR  $s \in \{-1, 1\}^{|A|}$  DO
  solutions := set of solutions of
   $\mathcal{A}_N^T (\mathcal{A}_B^{-1})^T \Phi_B \text{diag}(s_B) (\mathcal{A}_B^{-1}(q^{\text{nom}} - \mathcal{A}_N z))^2 = \Phi_N \text{diag}(s_N) z^2$ 
  FOR  $\hat{z} \in$  solutions DO
    IF  $\text{diag}(s_B) (\mathcal{A}_B^{-1}(q^{\text{nom}} - \mathcal{A}_N \hat{z})) \geq 0$  AND  $\text{diag}(s_N) \hat{z} \geq 0$  AND
    equations (5.2) – (5.4) hold for  $\hat{z}$  DO
      RETURN True
RETURN False

```

The following lemma gives an equivalent formulation of equation (5.1).

Lemma 5.3. *Equation (5.1) is equivalent to*

$$\sum_{\substack{b=(u,v) \\ \in A(\mathcal{C}_a) \setminus \{a\}}} \phi_b \left| \sum_{w \in D_{\mathcal{T}}(v)} q_w^{\text{nom}} - \sum_{c_c: \mathcal{C} \in \mathcal{C}_b} Q_{0,c_c} \right| \left(\sum_{w \in D_{\mathcal{T}}(v)} q_w^{\text{nom}} - \sum_{c_c: \mathcal{C} \in \mathcal{C}_b} Q_{0,c_c} \right) \quad (5.7)$$

$$= \phi_a |Q_{0,a}| Q_{0,a} \quad \text{for all } a \in A(\bar{\mathcal{T}}).$$

Proof. Since $\mathcal{A}_B^{-1} \mathcal{A}_N = -\mathcal{B}_B$ by Proposition 3.6, since the spanning tree \mathcal{T} of graph G is constructed with the DFS-Algorithm 3.1, and due to the orientation \vec{G} of graph G , all entries of $\mathcal{A}_B^{-1} \mathcal{A}_N$ are 0 or 1. Thus, multiplication of $\Phi_B | \mathcal{A}_B^{-1} q^{\text{nom}} - \mathcal{A}_B^{-1} \mathcal{A}_N Q_{0,N} | (\mathcal{A}_B^{-1} q^{\text{nom}} - \mathcal{A}_B^{-1} \mathcal{A}_N Q_{0,N})$ by $(\mathcal{A}_B^{-1} \mathcal{A}_N)^T$ means that in the row of (5.1) that corresponds to arc $a \in A(\bar{\mathcal{T}})$ not belonging to the spanning tree the components of $\Phi_B | \mathcal{A}_B^{-1} q^{\text{nom}} - \mathcal{A}_B^{-1} \mathcal{A}_N Q_{0,N} | (\mathcal{A}_B^{-1} q^{\text{nom}} - \mathcal{A}_B^{-1} \mathcal{A}_N Q_{0,N})$ are added that correspond to the spanning-tree arcs in the fundamental cycle \mathcal{C}_a . Hence, (5.1) is equivalent to

$$\sum_{\substack{b=(u,v) \\ \in A(\mathcal{C}_a) \setminus \{a\}}} \phi_b \left| (\mathcal{A}_B^{-1} q^{\text{nom}} - \mathcal{A}_B^{-1} \mathcal{A}_N Q_{0,N})_b \right| (\mathcal{A}_B^{-1} q^{\text{nom}} - \mathcal{A}_B^{-1} \mathcal{A}_N Q_{0,N})_b$$

$$= \phi_a |Q_{0,a}| Q_{0,a} \quad \text{for all } a \in A(\bar{\mathcal{T}}).$$

Since $\mathcal{A}_B^{-1} = \mathcal{P}$ due to Proposition 3.7, since the spanning tree \mathcal{T} of graph G is constructed with the DFS-Algorithm 3.1, and due to the orientation \vec{G} of graph G , all entries of \mathcal{A}_B^{-1} are 0 or 1, and thus, for all arcs $a \in A(\mathcal{T})$ the loads of

nodes $u \in V$ with $a \in A(r\mathcal{T}u)$ are summed up in $(\mathcal{A}_B^{-1}q^{\text{nom}})_a$. By the definition of descendants this yields

$$(\mathcal{A}_B^{-1}q^{\text{nom}})_a = \sum_{w \in D_{\mathcal{T}}(v)} q_w^{\text{nom}} \quad \text{for all } a = (u, v) \in A(\mathcal{T}).$$

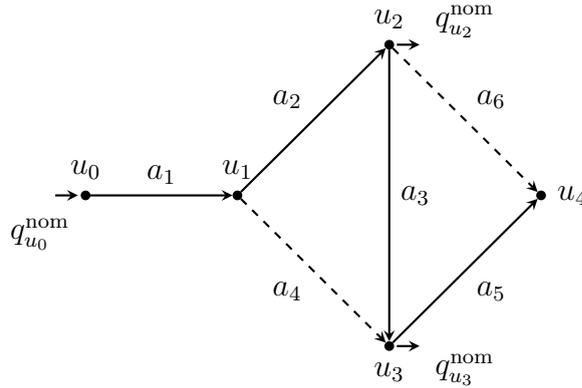
Finally, multiplying $Q_{0,N}$ by the row of $\mathcal{A}_B^{-1}\mathcal{A}_N$ that correspond to some spanning-tree arc $a \in A(\mathcal{T})$ sums up the flow along the arcs not belonging to the spanning tree that generate the fundamental cycles $\mathcal{C} \in C_{\mathcal{T}}$ with $a \in A(\mathcal{C})$ and hence

$$(\mathcal{A}_B^{-1}\mathcal{A}_N Q_{0,N})_a = \sum_{b_{\mathcal{C}}: \mathcal{C} \in C_a} Q_{0,b_{\mathcal{C}}}.$$

Altogether, this implies the assertion. \square

Let s_1 and s_2 be two vectors in the set $\{-1, 1\}^{|A|}$ of resolvings of the absolute values that coincide in all components corresponding to arcs that are contained in some cycle and differ only in components corresponding to arcs that are not contained in a cycle. Then Lemma 5.3 implicates that only one of these two resolvings of the absolute values has to be considered, because the equivalent formulation (5.7) of (5.1) does not contain components of s_1 and s_2 that correspond to arcs that are not contained in a cycle. This means that instead of all $2^{|A|}$ resolvings of the absolute values, only $2^{|\cup_{\mathcal{C} \in C} A(\mathcal{C})|}$ have to be considered. In Section 5.2 it will be shown that this number can be reduced further.

Example 5.4. Consider the following network.



The network contains one entry node, u_0 , and two exit nodes, u_2 and u_3 . The arcs not belonging to the spanning tree \mathcal{T} are depicted in dashed lines, $A(\overline{\mathcal{T}}) = \{a_4, a_6\}$. There are two fundamental cycles. One consisting of the arcs a_2 , a_3 and a_4 , the other one consisting of the arcs a_3 , a_5 and a_6 . Hence, system (5.1) consists of two equations having the form

$$\begin{aligned} \phi_{a_2} |Q_{0,a_2}| (Q_{0,a_2}) + \phi_{a_3} |Q_{0,a_3}| (Q_{0,a_3}) &= \phi_{a_4} |Q_{0,a_4}| Q_{0,a_4} \\ \phi_{a_3} |Q_{0,a_3}| (Q_{0,a_3}) + \phi_{a_5} |Q_{0,a_5}| (Q_{0,a_5}) &= \phi_{a_6} |Q_{0,a_6}| Q_{0,a_6}. \end{aligned}$$

Arc a_2 is only contained in the first fundamental cycle and the set of descendants of $u_2 = \text{head}(a_2)$ is $D_{\mathcal{T}}(u_2) = \{u_2, u_3, u_4\}$. Thus,

$$Q_{0,a_2} = q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} + q_{u_4}^{\text{nom}} - Q_{0,a_4} = q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4}.$$

Arc a_3 is contained in both fundamental cycles and the set of descendants of the head of a_3 is $D_{\mathcal{T}}(u_3) = \{u_3, u_4\}$, which leads to

$$Q_{0,a_3} = q_{u_3}^{\text{nom}} + q_{u_4}^{\text{nom}} - Q_{0,a_4} - Q_{0,a_6} = q_{u_3}^{\text{nom}} - Q_{0,a_4} - Q_{0,a_6}.$$

The flow along arc a_5 can be determined similarly. Altogether, this yields

$$\begin{aligned} & \phi_{a_2} \left| q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4} \right| \left(q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4} \right) \\ & + \phi_{a_3} \left| q_{u_3}^{\text{nom}} - Q_{0,a_4} - Q_{0,a_6} \right| \left(q_{u_3}^{\text{nom}} - Q_{0,a_4} - Q_{0,a_6} \right) = \phi_{a_4} |Q_{0,a_4}| Q_{0,a_4} \\ & \phi_{a_3} \left| q_{u_3}^{\text{nom}} - Q_{0,a_4} - Q_{0,a_6} \right| \left(q_{u_3}^{\text{nom}} - Q_{0,a_4} - Q_{0,a_6} \right) \\ & \quad + \phi_{a_5} | -Q_{0,a_6} | (-Q_{0,a_6}) = \phi_{a_6} |Q_{0,a_6}| Q_{0,a_6}. \end{aligned}$$

The section concludes with two properties of the set M of feasible load vectors.

Theorem 5.5. *The set M of feasible load vectors is bounded.*

Proof. Consider a sequence $(q_n^{\text{nom}+})_{n \in \mathbb{N}}$ of balanced load vectors in M with $\|q_n^{\text{nom}+}\|_2 \rightarrow \infty$ for $n \rightarrow \infty$. Then there exists an index i with $e_{u_i}^T q_n^{\text{nom}+} \rightarrow \infty$ or $e_{u_i}^T q_n^{\text{nom}+} \rightarrow -\infty$ for $n \rightarrow \infty$ and since each load vector has to be balanced, there exists an index i with $e_{u_i}^T q_n^{\text{nom}+} \rightarrow \infty$ and an index j with $e_{u_j}^T q_n^{\text{nom}+} \rightarrow -\infty$ for $n \rightarrow \infty$. Node u_i is an exit node of the network. Since there are only finitely many arcs that are incident to node u_i , the flow along at least one of those arcs, say arc a , has to flow towards the exit u_i . In addition, this flow has to fulfill $|(Q_{0,a})_n| (Q_{0,a})_n \rightarrow \infty$ for $n \rightarrow \infty$. By (4.9) this implies $e_{u_i}^T p_n \rightarrow 0$ for $n \rightarrow \infty$ and hence, for \hat{n} big enough, the pressure $e_{u_i}^T p_n$ at node u_i violates the lower pressure bound \underline{p}_{u_i} for $n > \hat{n}$. Thus, M is bounded. \square

Theorem 5.6. *The set M of feasible load vectors is closed.*

Proof. Consider a sequence $(q_n^{\text{nom}+})_{n \in \mathbb{N}}$ of balanced load vectors in M with $q_n^{\text{nom}+} \rightarrow \hat{q}^{\text{nom}+}$ for $n \rightarrow \infty$. It has to be shown that $\hat{q}^{\text{nom}+} \in M$ holds. Obviously, $\hat{q}^{\text{nom}+}$ is balanced.

As already mentioned, for a given load vector there exists a uniquely determined flow along the arcs yielding a sequence $(z_n)_{n \in \mathbb{N}}$. Now, assume $\|z_n\|_2 \rightarrow \infty$ for $n \rightarrow \infty$. Then there exists an index i with $e_{a_i}^T z_n \rightarrow \infty$ or $e_{a_i}^T z_n \rightarrow -\infty$ for $n \rightarrow \infty$. By the same reasons as in the previous proof it follows that $q_n^{\text{nom}+} \notin M$ for $n > \hat{n}$ and \hat{n} big enough, which is a contradiction. Hence, the sequence $(z_n)_{n \in \mathbb{N}}$ is bounded. It follows that there is a $\hat{z} \in \mathbb{R}^{|A|}$ with $z_n \rightarrow \hat{z}$ for $n \rightarrow \infty$.

Since the map $\mathcal{F}^* : \mathbb{R}^{|V|} \times \mathbb{R}^{|A(\overline{\mathcal{T}})|} \rightarrow |A(\overline{\mathcal{T}})|$ defined

$$(q^{\text{nom}}, z) \mapsto \Phi_N |z| z - \mathcal{A}_N^T g(q^{\text{nom}}, z)$$

is continuous,

$$\mathcal{F}^*(q_n^{\text{nom}}, z_n) = 0 \quad \text{for all } n$$

implies

$$\mathcal{F}^*(\hat{q}^{\text{nom}}, \hat{z}) = 0. \quad (5.8)$$

Moreover, the sequence $(z_n)_{n \in \mathbb{N}}$ of flows along the pipes implies a sequence $(p_n)_{n \in \mathbb{N}}$ of pressures at the nodes. By equation (4.13) the pressure depends continuously on the flow and hence, $p_n \rightarrow \hat{p}$ for $n \rightarrow \infty$, where \hat{p} is the pressure corresponding to flow \hat{z} . Again by continuity, $p_n \in [\underline{p}^+, \bar{p}^+]$ for all n leads to $\hat{p} \in [\underline{p}^+, \bar{p}^+]$. Together with (5.8) this implies $\hat{q}^{\text{nom}} \in M$ and hence M is closed. \square

In general, the set M of feasible load vectors is not convex.

5.2 Fixation of the Flow Direction

Since the resolving of the absolute values in system (5.1) corresponds to the flow direction along the pipes, the number of systems to be solved can be reduced if the flow direction along some pipes can be fixed and if combinations of flow directions can be excluded.

Proposition 5.7. *Let G be a graph representing a given network, \mathcal{T} a DFS-tree rooted in the reference node r oriented w.r.t. the predecessor function, \vec{G} the orientation of G w.r.t. the spanning tree \mathcal{T} , and Q_0 a flow on \vec{G} with corresponding pressure p^+ fulfilling (4.11) and (4.12). Assume $q_u^{\text{nom}} < 0$ for all entry nodes $u \in V_+$ and $q_u^{\text{nom}} > 0$ for all exit nodes $u \in V_-$. Then the following holds*

- (i) $\deg_{\text{gas}}^{\text{out}}(u) \geq 1$ for all entry nodes $u \in V_+$.
- (ii) $\deg_{\text{gas}}^{\text{in}}(u) \geq 1$ for all exit nodes $u \in V_-$.
- (iii) $\deg_{\text{gas}}^{\text{out}}(u) \geq 1$ and $\deg_{\text{gas}}^{\text{in}}(u) \geq 1$ (or $\deg_{\text{gas}}(u) = 0$) for all innodes $u \in V_0$.
- (iv) There are no cycles in \vec{G} that are directed w.r.t. the gas flow.

Moreover, if r is the only entry node of \vec{G} , then

- (v) The flow along arcs that do not belong to a cycle is directed away from the entry node r .
- (vi) Let $\vec{G}' = (V', A')$ where $V' := \{u \in V(\vec{G}) : \exists \mathcal{C} \in C \text{ with } u \in V(\mathcal{C})\}$ and $A' := \{a \in A(\vec{G}) : \exists \mathcal{C} \in C \text{ with } a \in A(\mathcal{C})\}$ and \mathcal{K} a component of \vec{G}' . Then node $u \in V(\mathcal{K})$ is an entry node of component \mathcal{K} if $u = r$ or $u = \text{head}(a)$ for some $a \in A(\vec{G}) \setminus A'$, and an exit node of component \mathcal{K} if $u = \text{tail}(a)$ for some $a \in A(\vec{G}) \setminus A'$ and there is no $b \in A(\vec{G}) \setminus A'$ with $u = \text{head}(b)$. Moreover, w.r.t. the subgraph \mathcal{K} of \vec{G}' the component \mathcal{K} has exactly one entry node \hat{r} and $\deg_{\text{gas}}^{\text{in}}(\hat{r}) = 0$.

A flow direction indicated by a flow on \vec{G} fulfilling (i) – (vi) is called a feasible flow direction for \vec{G} .

Proof. (i) Assume that there is some node $u \in V_+$ with $\deg_{\text{gas}}^{\text{out}}(u) = 0$. Let $a \in A(\vec{G})$ be an arc. Then $(\mathcal{A}^+)_{u,a} = 0$ if arc a is not incident to node u and thus $(\mathcal{A}^+)_{u,a} Q_{0,a} = 0$. If arc a is incident to node u and node u is the tail of arc a , then $(\mathcal{A}^+)_{u,a} = -1$ and $Q_{0,a} \leq 0$. If arc a is incident to node u and node u is the head of arc a , then $(\mathcal{A}^+)_{u,a} = 1$ and $Q_{0,a} \geq 0$. In both cases $(\mathcal{A}^+)_{u,a} Q_{0,a} \geq 0$ is valid. Since $q_u^{\text{nom}} < 0$ holds, there has to be at least one $\hat{a} \in A$ with $(\mathcal{A}^+)_{u,\hat{a}} Q_{0,\hat{a}} > 0$. This yields the contradiction

$$0 < (\mathcal{A}^+)_{u,\bullet} Q_0 = q_u^{\text{nom}} < 0.$$

(ii) Equivalently to the proof of (i) one gets the contradiction

$$0 > (\mathcal{A}^+)_{u,\bullet} Q_0 = q_u^{\text{nom}} > 0.$$

(iii) Analogous to (i) and (ii).

(iv) Assume that there is a cycle $u_1, a_1, u_2, a_2, \dots, a_n, u_{n+1}$ with $u_{n+1} = u_1$ in that the gas flow is directed from u_i to u_{i+1} for $i = 1, \dots, n$ and that there is at least one arc a in the cycle with $Q_{0,a} \neq 0$. For $i = 1, \dots, n$, if $a_i = (u_i, u_{i+1})$, then $(p_{u_{i+1}})^2 - (p_{u_i})^2 = -\phi_{a_i} |Q_{0,a_i}| Q_{0,a_i}$ by equation (4.9). Since $Q_{0,a_i} \geq 0$ in this case, $(p_{u_{i+1}})^2 - (p_{u_i})^2 \leq 0$.

If $a_i = (u_{i+1}, u_i)$, then $(p_{u_i})^2 - (p_{u_{i+1}})^2 = -\phi_{a_i} |Q_{0,a_i}| Q_{0,a_i}$ by equation (4.9) and since $Q_{0,a_i} \leq 0$ in this case, $(p_{u_i})^2 - (p_{u_{i+1}})^2 \geq 0$. Multiplying this inequality by -1 yields $(p_{u_{i+1}})^2 - (p_{u_i})^2 \leq 0$.

Together with $Q_{0,a} \neq 0$ for at least one arc a in the cycle one gets

$$0 = \sum_{i=1}^n (p_{u_{i+1}})^2 - (p_{u_i})^2 < 0$$

which is a contradiction.

(v) Let $a \in A(\vec{G})$ be an arc that does not belong to a cycle. Hence, arc a is an arc of the spanning tree and therefore

$$Q_{0,a} = (\mathcal{A}_B^{-1} q^{\text{nom}})_a - (\mathcal{A}_B^{-1} \mathcal{A}_N Q_{0,N})_a.$$

Since $\mathcal{A}_B^{-1} = \mathcal{P}$ by Proposition 3.7, since the spanning tree \mathcal{T} of graph G is constructed with the DFS-Algorithm 3.1, and due to the orientation \vec{G} of graph G , all entries of \mathcal{A}_B^{-1} are 0 or 1. Moreover, $q^{\text{nom}} \geq 0$ because the reference node is the only entry node and thus $\mathcal{A}_B^{-1} q^{\text{nom}} \geq 0$.

By definition of the cycle matrix \mathcal{B} and since $\mathcal{A}_B^{-1} \mathcal{A}_N = -\mathcal{B}_B$ due to Proposition 3.6, $(\mathcal{A}_B^{-1} \mathcal{A}_N)_{a,\bullet} = (0, \dots, 0)$ holds and hence $(\mathcal{A}_B^{-1} \mathcal{A}_N Q_{0,N})_a = 0$.

Altogether, this yields $Q_{0,a} \geq 0$ and since the arc a is directed by the DFS-Algorithm 3.1, the flow along arc a is directed away from r .

(vi) Let $u \in V(\mathcal{K})$ be a node in component \mathcal{K} with $u = \text{head}(a)$ for some arc $a \in A(\vec{G}) \setminus A'$. Together with the flow direction of the gas along arc a by (v) this implies

$$Q_{0,a} = \sum_{v \in D_{\mathcal{T}}(u)} \underbrace{q_v^{\text{nom}}}_{\geq 0} \geq q_u^{\text{nom}} + \sum_{\substack{v \in D_{\mathcal{T}}(u): \\ A(u\mathcal{T}v) \cap A' = \emptyset}} q_v^{\text{nom}} = q_u^{\text{nom}} + \sum_{\substack{b \in A(\vec{G}) \setminus A': \\ u = \text{tail}(b)}} Q_{0,b}.$$

Now, one gets

$$q_u^{\text{nom}} = \mathcal{A}_{u,\bullet}^+ Q_0 = Q_{0,a} - \sum_{\substack{b \in A(\vec{G}) \setminus A': \\ u = \text{tail}(b)}} Q_{0,b} + (\mathcal{A}_{u,\bullet}^+)_{\mathcal{K}} (Q_0)_{\mathcal{K}}.$$

Therefore, the load of node u w.r.t. component \mathcal{K} is

$$q_u^{\text{nom}} + \sum_{\substack{b \in A(\vec{G}) \setminus A': \\ u = \text{tail}(b)}} Q_{0,b} - Q_{0,a} \leq 0$$

and it follows that node u is an entry node w.r.t. component \mathcal{K} .

In the same way it can be concluded, that a node $u \in V(\mathcal{K})$ such that $u = \text{tail}(a)$ for some $a \in A(\vec{G}) \setminus A'$ and there is no $a \in A(\vec{G}) \setminus A'$ with $u = \text{head}(a)$ is an exit node w.r.t. component \mathcal{K} .

To show that the component \mathcal{K} has exactly one entry node w.r.t. the subgraph, assume that \mathcal{K} contains two entry nodes u and v w.r.t. the subgraph. If \mathcal{K} contains the entry node r of \vec{G} , then, w.l.o.g., let $u = r$. The other entry node of \mathcal{K} , v , has to be the head of an arc $a \in A(\vec{G}) \setminus A'$ and thus, arc a is directed toward the entry node r of \vec{G} , which contradicts the fact that the spanning tree \mathcal{T} is directed w.r.t. the predecessor function of the DFS-Algorithm 3.1. If \mathcal{K} does not contain the entry node r of \vec{G} , then u and v are heads of arcs $a, b \in A(\vec{G}) \setminus A'$, respectively. Since \vec{G} is connected, there exists a path $r\mathcal{T}u$ connecting r and u . Since arc a is not contained in a cycle, it has to be contained in this path. For the same reasons there exists a path $r\mathcal{T}v$ connecting r and v containing b . Finally, there is a path $u\mathcal{T}v$ in \mathcal{K} connecting u and v . This results in the cycle $r\mathcal{T}u, u\mathcal{T}v, v\mathcal{T}r$ containing the arcs a and b , which contradicts $a, b \in A(\vec{G}) \setminus A'$.

Now suppose that \mathcal{K} does not have any entry node w.r.t. the subgraph, i.e., \mathcal{K} does not contain the head of an arc in $A(\vec{G}) \setminus A'$. Then \mathcal{K} has to contain the tail of an arc $a \in A(\vec{G}) \setminus A'$ that is part of a way connecting the root node r and the component \mathcal{K} since \vec{G} is connected. But this contradicts the fact that the spanning tree \mathcal{T} is directed w.r.t. the predecessor function of the DFS-Algorithm 3.1. Thus, component \mathcal{K} contains the head u of some arc $a \in A(\vec{G}) \setminus A'$, i.e., node u is an entry node w.r.t. component \mathcal{K} .

Hence, the component \mathcal{K} has a unique entry node \hat{r} w.r.t. the subgraph. It remains to show that $\deg_{\text{gas}}^{\text{in}}(\hat{r}) = 0$ holds. Since all arcs in component \mathcal{K} are contained in cycles and graph \vec{G} is connected, there have to be at least two arcs that are incident to \hat{r} . Assume that there is an arc incident to \hat{r} along that gas is flowing towards \hat{r} . Backtrack this gas flow along one of its ways as long as possible. Then this way cannot contain cycles, because then there would be a cycle that is directed w.r.t. the gas flow, in contradiction to (iv). Let u be the end node of this way. Then u cannot be an entry node of component \mathcal{K} since there is only one entry node in \mathcal{K} and because the way started in this entry node, it would lead to a cycle directed w.r.t. the gas flow if $u = \hat{r}$ would hold. But since $\deg_{\text{gas}}^{\text{in}}(u) = 0$ it cannot be an exit node or innode neither. This proves the claim that $\deg_{\text{gas}}^{\text{in}}(\hat{r}) = 0$. \square

Remark 5.8. In networks with more than one entry node the flow along arcs that do not belong to a cycle cannot be directed in advance for arbitrary loads. However, if the loads are fixed, fixation of the flow direction along the arcs not belonging to a cycle is possible: Consider the graph G representing a network with several entry nodes, a load vector $q^{\text{nom}+}$ and an edge $a = \{u, v\} \in A$ that does not belong to any cycle in G . Let $G' = (V(G), A(G) \setminus \{a\})$ be the graph where edge a is deleted. Then G' consists of two components. Let \mathcal{K}_u be the component containing node u and \mathcal{K}_v be the component containing node v . If

$$\sum_{w \in V(\mathcal{K}_u)} q_w^{\text{nom}} < 0,$$

then it has to hold

$$\sum_{w \in V(\mathcal{K}_v)} q_w^{\text{nom}} > 0,$$

because the load is balanced, and along edge a the gas has to flow from node u to node v . If

$$\sum_{w \in V(\mathcal{K}_u)} q_w^{\text{nom}} > 0,$$

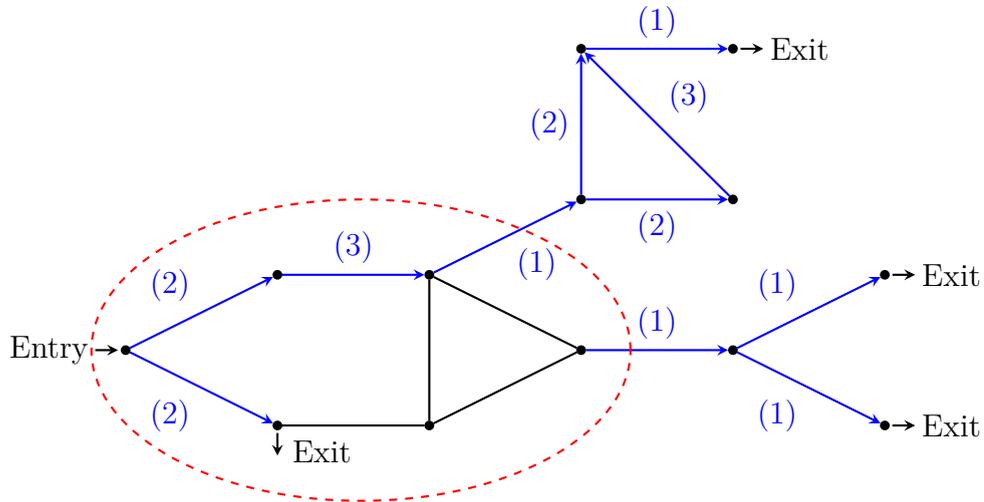
then

$$\sum_{w \in V(\mathcal{K}_v)} q_w^{\text{nom}} < 0$$

holds and thus along edge a the gas has to flow from node v to node u . If both sums are zero, there is no gas flow along edge a .

Example 5.9 illustrates the usage of Proposition 5.7.

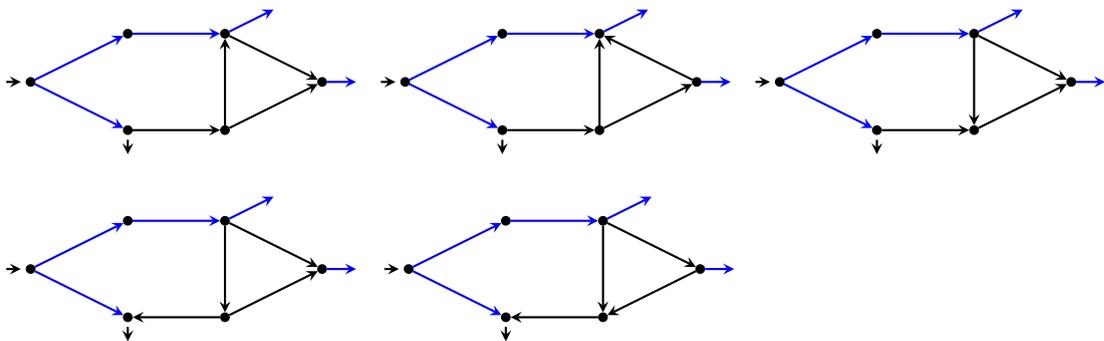
Example 5.9. Consider the following network with one entry node and four exit nodes. The small numbers in brackets indicate in which step the flow direction has been fixed.



The network contains exactly one entry node and thus by (v) of Proposition 5.7, the flow along arcs that do not belong to a cycle is directed away from the entry node, indicated by (1).

After deletion of these five arcs the network decomposes into two components each having exactly one entry node and by (vi) of Proposition 5.7 the flow along the arcs incident to these two entry nodes has to be directed away from the particular entry node. Arcs along which the flows are directed in this step are indicated by (2). By (iii) of Proposition 5.7 the two arcs labeled (3) have to be directed in the way depicted in the figure.

There are only four arcs of the 15 arcs where the flow direction cannot be fixed. But there are still some combinations of flow directions that are not feasible because they violate some of the rules in Proposition 5.7, so that not all of the $2^4 = 16$ flow directions have to be checked. In the following only the part of the figure encircled by the red dashed line is considered. The graphs depicted below show all feasible flow directions in this part of the original network.



In Figure A.1 in Appendix A.1 the flow directions violating the rules in Proposition 5.7 are shown. Moreover, the reasons for infeasibility of those flow directions are given there.

This means that instead of originally $2^{15} = 32,768$ flow directions there remain only five feasible flow directions.

Some numerical results of this procedure are shown in Table 6.2 in Section 6.2.

5.2.1 Upper Bounds for the Number of Flow Directions

In a tree structured network with exactly one entry node the flow direction is uniquely determined and independent of the actual load vector by (v) of Proposition 5.7. In tree structured networks with more than one entry node the flow direction depends on the actual load vector, but can be uniquely determined if some load vector is given, see Remark 5.8.

In case the network contains exactly one entry node and consists of exactly one fundamental cycle, the number of feasible flow directions of the gas can be given exactly, too.

Theorem 5.10. *Let G be a graph representing a network that consists of exactly one cycle, i.e., there is no edge that does not belong to this cycle. Let r be the only entry node in G and assume $q_u^{\text{nom}} > 0$ for all exit nodes $u \in V_-$. Then there are exactly $|V_-|$ feasible flow directions of the gas along the edges in graph G .*

Proof. By (vi) of Proposition 5.7, it holds $\deg_{\text{gas}}^{\text{in}}(r) = 0$. Hence, there has to be exactly one exit node $u \in V_-$ such that $\deg_{\text{gas}}^{\text{in}}(u) = 2$, $\deg_{\text{gas}}^{\text{out}}(u) = 0$, $\deg_{\text{gas}}^{\text{in}}(v) = 1$, and $\deg_{\text{gas}}^{\text{out}}(v) = 1$ for all $v \in V \setminus \{u\}$, because otherwise there would be a node $w \in V$ with $\deg_{\text{gas}}^{\text{in}}(w) = 0$, which contradicts (ii) and (iii) of Proposition 5.7. Since exit node u is arbitrary, the assertion is proven. \square

If the network consists of two or more fundamental cycles that are not edge-disjoint and there are no arcs that do not belong to any cycle, some fundamentals of hyperplane arrangements have to be exploited, see e.g., [35, 101].

Let G be the graph representing a given network, \mathcal{T} a DFS-tree rooted in the reference node r oriented w.r.t. the predecessor function, and \vec{G} the orientation of G w.r.t the spanning tree \mathcal{T} . With each arc $a \in A$ there can be identified a hyperplane \mathcal{H}_a where

$$\mathcal{H}_a := \begin{cases} \{Q_{0,N} : Q_{0,a} = 0\} & \text{if } a \in A(\vec{\mathcal{T}}), \\ \{Q_{0,N} : \sum_{u \in D_{\mathcal{T}}(\text{head}(a))} q_u^{\text{nom}} - \sum_{b \in C_a} Q_{0,b} = 0\} & \text{else.} \end{cases}$$

The connected components of $\mathbb{R}^{|A(\vec{\mathcal{T}})|} \setminus \bigcup_{a \in A} \mathcal{H}_a$ are called regions of the set of hyperplanes. Each feasible flow direction can be uniquely mapped to one of these regions and hence, the number of those regions is an upper bound for the number of feasible flow directions. In [101] it is shown that the number of regions equals

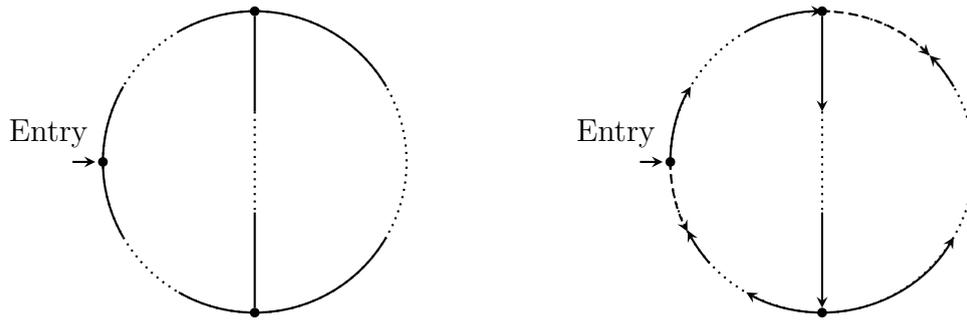
$$(-1)^{|A(\vec{\mathcal{T}})|} \sum_{\substack{H \subseteq \{\mathcal{H}_a : a \in A\}, \\ \bigcap_{\mathcal{H} \in H} \mathcal{H} \neq \emptyset}} (-1)^{|H|} (-1)^{|A(\vec{\mathcal{T}})| - \text{rank}(H)} \quad (5.9)$$

where $\text{rank}(H)$ is the dimension of the space spanned by the normals to the hyperplanes in H .

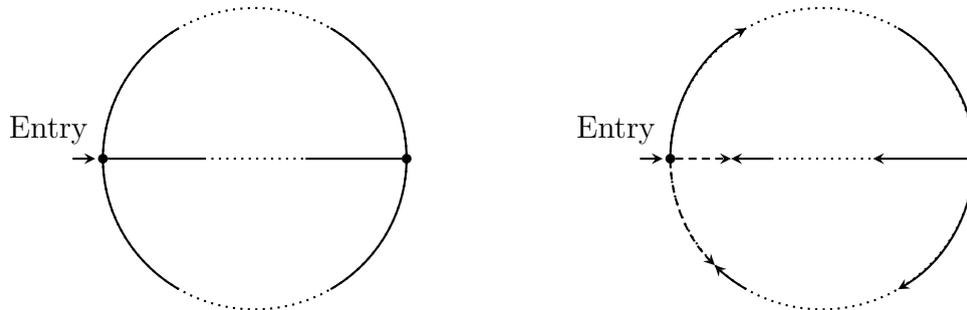
If the network consists of exactly two fundamental cycles that are not edge-disjoint, the sets $H \subseteq \{\mathcal{H}_a : a \in A\}$ with $\bigcap_{\mathcal{H} \in H} \mathcal{H} \neq \emptyset$ can be fully characterized.

5.2.1.1 Exactly Two Interconnected Fundamental Cycles

Figure 5.1 shows the two different types of graphs that are possible if only networks are considered that consist of exactly two fundamental cycles that are not edge-disjoint, contain no arcs that do not belong to any cycle, and contain exactly one entry node. The dotted lines in the figure indicate that there can be an arbitrary number of arcs on the bows. On the right side, the DFS-trees of the graphs are depicted where the dashed lines are the arcs of the cotree. The arcs represented by the dotted lines are oriented in the same direction as the solid lines they are framed by. The DFS-trees are unique up to graphical representation.



(a) Type 1, on the right with DFS-tree.



(b) Type 2, on the right with DFS-tree.

Figure 5.1: Possible types of networks consisting of exactly two fundamental cycles and their DFS-trees that are unique up to graphical representation.

Since only networks with two fundamental cycles are considered, let $A(\overline{\mathcal{T}}) = \{a_1, a_2\}$. Then there are three different types of hyperplanes:

1. hyperplanes parallel to the Q_{0,a_1} -axis,
2. hyperplanes parallel to the Q_{0,a_2} -axis,
3. hyperplanes intersecting the axes in the points $(t, 0)$ and $(0, t)$ for some $t \in \mathbb{R}_{>0}$.

The following three lemmata provide a crucial contribution to the desired characterization of the sets $H \subseteq \{\mathcal{H}_a : a \in A\}$ with $\bigcap_{\mathcal{H} \in H} \mathcal{H} \neq \emptyset$.

Lemma 5.11. *Let G be the graph representing a given network, \mathcal{T} a DFS-tree rooted in the reference node r oriented w.r.t. the predecessor function, and \vec{G} the orientation of G w.r.t the spanning tree \mathcal{T} . Let r be the only entry node in \vec{G} and assume $q_u^{\text{nom}} > 0$ for all exit nodes $u \in V_-$ and that there are no innodes in the network, i.e., $V_0 = \emptyset$. Consider two arcs $a, b \in A$, $a \neq b$, with $C_a = C_b$. Then the hyperplanes \mathcal{H}_a and \mathcal{H}_b are parallel but not identical.*

Proof. Let a and b be both in $A(\mathcal{T})$. W.l.o.g. assume that a was found before b during the DFS-Algorithm 3.1. Because a and b are contained in exactly the same fundamental cycles, there has to be a directed path $\text{head}(a)\mathcal{T}\text{head}(b)$ in \mathcal{T} and there exists a node that is descendant of $\text{head}(a)$ and proper ancestor of $\text{head}(b)$. This yields $D_{\mathcal{T}}(\text{head}(a)) \supset D_{\mathcal{T}}(\text{head}(b))$ and hence,

$$\sum_{u \in D_{\mathcal{T}}(\text{head}(a))} q_u^{\text{nom}} > \sum_{u \in D_{\mathcal{T}}(\text{head}(b))} q_u^{\text{nom}}.$$

Moreover, since a and b are contained in exactly the same fundamental cycles,

$$\sum_{c_c: C \in C_a} Q_{0,c_c} = \sum_{c_c: C \in C_b} Q_{0,c_c}$$

holds. Altogether, this implies that the hyperplanes

$$\mathcal{H}_a = \left\{ Q_{0,N}: \sum_{u \in D_{\mathcal{T}}(\text{head}(a))} q_u^{\text{nom}} - \sum_{c_c: C \in C_a} Q_{0,c_c} = 0 \right\}$$

and

$$\mathcal{H}_b = \left\{ Q_{0,N}: \sum_{u \in D_{\mathcal{T}}(\text{head}(b))} q_u^{\text{nom}} - \sum_{c_c: C \in C_b} Q_{0,c_c} = 0 \right\}$$

are parallel but not identical.

Now, let a be in $A(\mathcal{T})$ and b be in $A(\overline{\mathcal{T}})$. Then both arcs are in exactly one fundamental cycle and the hyperplanes

$$\mathcal{H}_a = \left\{ Q_{0,N}: \underbrace{\sum_{u \in D_{\mathcal{T}}(\text{head}(a))} q_u^{\text{nom}}}_{>0} - Q_{0,b} = 0 \right\}$$

and

$$\mathcal{H}_b = \{Q_{0,N}: Q_{0,b} = 0\}$$

are parallel but not identical. \square

Lemma 5.12. *Let G be a graph representing a network consisting of exactly two fundamental cycles that are not edge-disjoint and containing no arcs that do not belong to any cycle, \mathcal{T} a DFS-tree rooted in the reference node r oriented w.r.t. the predecessor function, and \vec{G} the orientation of G w.r.t the spanning tree \mathcal{T} . Let r be the only entry node in \vec{G} and assume $q_u^{\text{nom}} > 0$ for all exit nodes $u \in V_-$ and that there are no innodes in the network, i.e., $V_0 = \emptyset$. Consider two arcs $a, b \in A$, $a \neq b$, with $C_a \neq C_b$. Then the hyperplanes \mathcal{H}_a and \mathcal{H}_b are not parallel.*

Proof. The assumption $C_a \neq C_b$ implies

$$\sum_{c_c: c \in C_a} Q_{0,c_c} \neq \sum_{c_c: c \in C_b} Q_{0,c_c}.$$

and hence, the hyperplanes \mathcal{H}_a and \mathcal{H}_b are not parallel. \square

Lemma 5.13. *Let G be a graph representing a network consisting of exactly two fundamental cycles that are not edge-disjoint and containing no arcs that do not belong to any cycle, \mathcal{T} a DFS-tree rooted in the reference node r oriented w.r.t. the predecessor function, and \vec{G} the orientation of G w.r.t the spanning tree \mathcal{T} . Let r be the only entry node in \vec{G} and assume $q_u^{\text{nom}} > 0$ for all exit nodes $u \in V_-$ and that there are no innodes in the network, i.e., $V_0 = \emptyset$. Then there is no point in \mathbb{R}^2 where more than two hyperplanes corresponding to the arcs in A intersect.*

Proof. Let $A(\overline{\mathcal{T}}) = \{a_1, a_2\}$. Since hyperplanes that belong to the same type of hyperplanes (see list above) are parallel but not identical, there can be at most three hyperplanes that intersect in one point, each of them belonging to a different type of hyperplanes. Let $\mathcal{H}_a, \mathcal{H}_b, \mathcal{H}_c$ denote these three hyperplanes corresponding to the three arcs a, b, c , respectively, and let \mathcal{H}_a belong to type 1, \mathcal{H}_b to type 2, and \mathcal{H}_c to type 3.

Assume that there is exactly one arc among a, b, c that is an element of $A(\overline{\mathcal{T}})$. Arc c belongs to two fundamental cycles and hence cannot be an arc of the cotree. W.l.o.g. let a be the arc in $A(\overline{\mathcal{T}})$, i.e., $a = a_1$. Then the three hyperplanes are

$$\begin{aligned} \mathcal{H}_a &= \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : Q_{0,a_1} = 0 \right\} \\ \mathcal{H}_b &= \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : \sum_{u \in D_{\mathcal{T}}(\text{head}(b))} q_u^{\text{nom}} - Q_{0,a_2} = 0 \right\} \\ \mathcal{H}_c &= \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : \sum_{u \in D_{\mathcal{T}}(\text{head}(c))} q_u^{\text{nom}} - Q_{0,a_1} - Q_{0,a_2} = 0 \right\} \end{aligned}$$

and the point where all three hyperplanes intersect has to fulfill

$$\sum_{u \in D_{\mathcal{T}}(\text{head}(b))} q_u^{\text{nom}} - \sum_{u \in D_{\mathcal{T}}(\text{head}(c))} q_u^{\text{nom}} = 0.$$

Since arcs b and c are both arcs of the spanning tree and b is contained in exactly one fundamental cycle whereas c is contained in exactly two fundamental cycles, Figure 5.1 shows that either $D_{\mathcal{T}}(\text{head}(b)) \subset D_{\mathcal{T}}(\text{head}(c))$ or $D_{\mathcal{T}}(\text{head}(b)) \supset D_{\mathcal{T}}(\text{head}(c))$. Hence, either

$$0 < \sum_{u \in D_{\mathcal{T}}(\text{head}(b))} q_u^{\text{nom}} < \sum_{u \in D_{\mathcal{T}}(\text{head}(c))} q_u^{\text{nom}}$$

or

$$\sum_{u \in D_{\mathcal{T}}(\text{head}(b))} q_u^{\text{nom}} > \sum_{u \in D_{\mathcal{T}}(\text{head}(c))} q_u^{\text{nom}} > 0$$

holds. This implies that there does not exist a point where all three hyperplanes \mathcal{H}_a , \mathcal{H}_b and \mathcal{H}_c intersect.

Now, assume that there are exactly two arcs among a , b , c that are elements of $A(\overline{\mathcal{T}})$. These two arcs have to be a and b which leads to the three hyperplanes

$$\begin{aligned}\mathcal{H}_a &= \{(Q_{0,a_1}, Q_{0,a_2})^T : Q_{0,a_1} = 0\} \\ \mathcal{H}_b &= \{(Q_{0,a_1}, Q_{0,a_2})^T : Q_{0,a_2} = 0\} \\ \mathcal{H}_c &= \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : \sum_{u \in D_{\mathcal{T}}(\text{head}(c))} q_u^{\text{nom}} - Q_{0,a_1} - Q_{0,a_2} = 0 \right\}.\end{aligned}$$

Since $\sum_{u \in D_{\mathcal{T}}(\text{head}(c))} q_u^{\text{nom}} > 0$, there is no point where all three hyperplanes \mathcal{H}_a , \mathcal{H}_b and \mathcal{H}_c intersect.

Finally, assume that all three arcs a , b , and c are arcs of the spanning tree. Hence, the three hyperplanes are

$$\begin{aligned}\mathcal{H}_a &= \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : \sum_{u \in D_{\mathcal{T}}(\text{head}(a))} q_u^{\text{nom}} - Q_{0,a_1} = 0 \right\}, \\ \mathcal{H}_b &= \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : \sum_{u \in D_{\mathcal{T}}(\text{head}(b))} q_u^{\text{nom}} - Q_{0,a_2} = 0 \right\}, \\ \mathcal{H}_c &= \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : \sum_{u \in D_{\mathcal{T}}(\text{head}(c))} q_u^{\text{nom}} - Q_{0,a_1} - Q_{0,a_2} = 0 \right\}\end{aligned}$$

and the point where all three hyperplanes intersect has to fulfill

$$\sum_{u \in D_{\mathcal{T}}(\text{head}(a))} q_u^{\text{nom}} + \sum_{u \in D_{\mathcal{T}}(\text{head}(b))} q_u^{\text{nom}} - \sum_{u \in D_{\mathcal{T}}(\text{head}(c))} q_u^{\text{nom}} = 0. \quad (5.10)$$

From Figure 5.1 it follows that there are two different orderings in that arcs a , b , and c can be found during DFS-Algorithm 3.1.

Case 1: a, c, b . This implies $D_{\mathcal{T}}(\text{head}(a)) \supset D_{\mathcal{T}}(\text{head}(c)) \supset D_{\mathcal{T}}(\text{head}(b))$ and hence, (5.10) becomes

$$0 < \sum_{\substack{u \in D_{\mathcal{T}}(\text{head}(a)) \setminus \\ D_{\mathcal{T}}(\text{head}(c))}} q_u^{\text{nom}} + \sum_{u \in D_{\mathcal{T}}(\text{head}(b))} q_u^{\text{nom}} = 0,$$

which is a contradiction.

Case 2: c, a, b . This implies $D_{\mathcal{T}}(\text{head}(a)) \subset D_{\mathcal{T}}(\text{head}(c))$, $D_{\mathcal{T}}(\text{head}(b)) \subset D_{\mathcal{T}}(\text{head}(c))$, and $D_{\mathcal{T}}(\text{head}(a)) \cap D_{\mathcal{T}}(\text{head}(b)) = \emptyset$. Thus, (5.10) becomes

$$0 > - \sum_{\substack{u \in D_{\mathcal{T}}(\text{head}(c)) \setminus \\ (D_{\mathcal{T}}(\text{head}(a)) \cup D_{\mathcal{T}}(\text{head}(b)))}} q_u^{\text{nom}} = 0,$$

what is not possible. □

Theorem 5.14. *Let G be a graph representing a network consisting of exactly two fundamental cycles that are not edge-disjoint and containing no arcs that do not belong to any cycle, \mathcal{T} a DFS-tree rooted in the reference node r oriented w.r.t. the predecessor function, \vec{G} the orientation of G w.r.t the spanning tree \mathcal{T} , and $A(\vec{\mathcal{T}}) = \{a_1, a_2\}$. Let r be the only entry node in \vec{G} and assume $q_u^{\text{nom}} > 0$ for all exit nodes $u \in V_-$ and that there are no innodes in the networks, i.e., $V_0 = \emptyset$. Set $\mathcal{P} := \{\mathcal{P}_1, \mathcal{P}_2, \mathcal{P}_3\} = \{\{\mathcal{C}_{a_1}\}, \{\mathcal{C}_{a_2}\}, \{\mathcal{C}_{a_1}, \mathcal{C}_{a_2}\}\}$. Then there are at most*

$$\sum_{i=2}^3 \left(|A_{\mathcal{P}_i}| \sum_{j=1}^{i-1} |A_{\mathcal{P}_j}| \right) + |A| + 1 \quad (5.11)$$

feasible flow directions of the gas along the arcs in \vec{G} .

It is an upper bound in the sense that it only takes into account (i) and (ii) of Proposition 5.7 and that every exit node needs to be served, i.e., there is a path from the entry node r to every exit node in the network that is directed w.r.t. the flow direction of the gas.

Proof. To verify correctness of formula (5.11) the sets $H \subseteq \{\mathcal{H}_a : a \in A\}$ with $\bigcap_{\mathcal{H} \in H} \mathcal{H} \neq \emptyset$ have to be characterized. Due to Lemma 5.13 the cardinality of a set H of hyperplanes whose intersection is not empty has to be smaller than three.

Setting $H = \emptyset$ yields

$$(-1)^{|H|} (-1)^{2-\text{rank}(H)} = (-1)^0 (-1)^{2-0} = 1. \quad (5.12)$$

Each hyperplane \mathcal{H}_a with $a \in A$ is nonempty and thus one gets

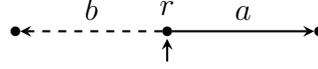
$$\sum_{\substack{H \subseteq \{\mathcal{H}_a : a \in A\}, \\ \bigcap_{\mathcal{H} \in H} \mathcal{H} \neq \emptyset, \\ |H|=1}} (-1)^{|H|} (-1)^{2-\text{rank}(H)} = |A| (-1)^1 (-1)^{2-1} = |A|. \quad (5.13)$$

Two distinct intersecting hyperplanes \mathcal{H}_a and \mathcal{H}_b have to correspond to two distinct arcs a and b with $C_a \neq C_b$ by Lemma 5.11. Moreover, every pair of hyperplanes \mathcal{H}_a and \mathcal{H}_b with $C_a \neq C_b$ intersects in exactly one point due to Lemma 5.12. This implies

$$\begin{aligned} & \sum_{\substack{H \subseteq \{\mathcal{H}_a : a \in A\}, \\ \bigcap_{\mathcal{H} \in H} \mathcal{H} \neq \emptyset, \\ |H|=2}} (-1)^{|H|} (-1)^{2-\text{rank}(H)} \\ &= (|A_{\mathcal{P}_1}| |A_{\mathcal{P}_2}| + |A_{\mathcal{P}_1}| |A_{\mathcal{P}_3}| + |A_{\mathcal{P}_2}| |A_{\mathcal{P}_3}|) (-1)^2 (-1)^{2-2} \\ &= |A_{\mathcal{P}_1}| |A_{\mathcal{P}_2}| + |A_{\mathcal{P}_1}| |A_{\mathcal{P}_3}| + |A_{\mathcal{P}_2}| |A_{\mathcal{P}_3}|. \end{aligned} \quad (5.14)$$

Summing up equations (5.12) – (5.14) and multiplying the result by $(-1)^{|A(\vec{\mathcal{T}})|} = (-1)^2 = 1$ yields the desired equality of equations (5.9) and (5.11).

To prove that the bound takes care of (i) of Proposition 5.7 assume that $\deg r = 2$. By Figure 5.1, one of the arcs incident to r is an arc in \mathcal{T} and one is an arc in $\overline{\mathcal{T}}$. Let $a \in A(\mathcal{T})$ and $b \in A(\overline{\mathcal{T}})$, w.l.o.g. $b = a_1$, be incident to node r . Then arcs a and b are both contained in fundamental cycle \mathcal{C}_{a_1} . Moreover, they are not contained in any other fundamental cycles. The direction of the arcs in \vec{G} is depicted in the following graphic.



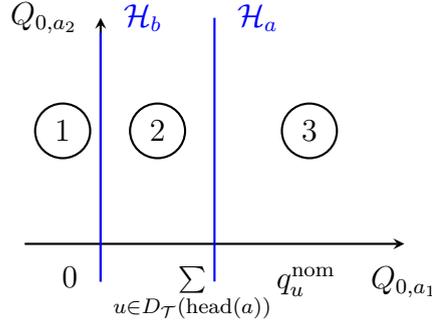
The hyperplanes corresponding to arcs a and b are

$$\mathcal{H}_a = \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : \sum_{u \in D_{\mathcal{T}}(\text{head}(a))} q_u^{\text{nom}} - Q_{0,a_1} = 0 \right\}$$

and

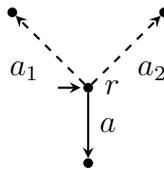
$$\mathcal{H}_b = \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : Q_{0,a_1} = 0 \right\}.$$

The two hyperplanes are parallel. Thus, there are three regions.



In region ① the flow along arc b is strictly negative and the flow along arc a is strictly positive and hence, $\deg_{\text{gas}}^{\text{in}}(r) = \deg_{\text{gas}}^{\text{out}}(r) = 1$. In region ② it holds $Q_{0,b} > 0$ and $Q_{0,a} > 0$. This implies $\deg_{\text{gas}}^{\text{out}}(r) = 2$ and $\deg_{\text{gas}}^{\text{in}}(r) = 0$. Finally, in region ③, the flow along arc b is directed away from node r and the flow along arc a is directed towards node r . Thus, if $\deg r = 2$, the out-degree w.r.t. the gas flow of node r is always greater than or equal to 1.

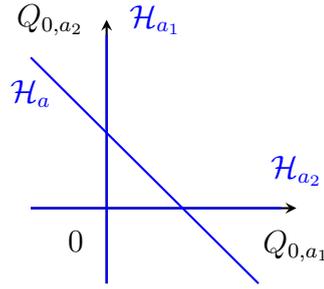
Now, assume $\deg r = 3$. Among the three arcs incident to node r there is exactly one tree-arc. Let $a \in A(\mathcal{T})$ denote this arc. The other two arcs are $a_1, a_2 \in A(\overline{\mathcal{T}})$. The direction of the arcs in \vec{G} is depicted in the following graphic.



The hyperplanes corresponding to arcs a , a_1 and a_2 are

$$\begin{aligned}\mathcal{H}_a &= \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : \sum_{u \in D_{\mathcal{T}}(\text{head}(a))} q_u^{\text{nom}} - Q_{0,a_1} - Q_{0,a_2} = 0 \right\}, \\ \mathcal{H}_{a_1} &= \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : Q_{0,a_1} = 0 \right\}, \\ \mathcal{H}_{a_2} &= \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : Q_{0,a_2} = 0 \right\}.\end{aligned}$$

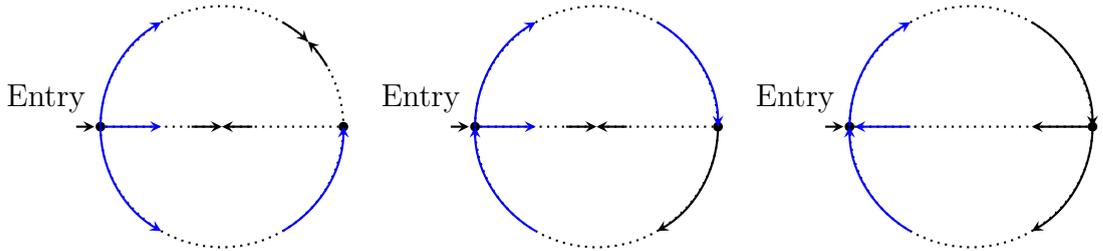
Thus, there are seven regions.



If $\text{deg}_{\text{gas}}^{\text{out}}(r) = 0$ holds, the flow along arcs a , a_1 and a_2 is negative. This implies that $(Q_{0,a_1}, Q_{0,a_2})^T$ has to be a point below of hyperplane \mathcal{H}_{a_2} , left of hyperplane \mathcal{H}_{a_1} and above of hyperplane \mathcal{H}_a . But obviously this is not possible and hence, $\text{deg}_{\text{gas}}^{\text{out}}(r) \geq 1$ holds.

The proof of the consideration of (ii) of Proposition 5.7 is carried out equivalently.

To show that every exit node is served the two types of networks in Figure 5.1 are discussed separately. First, consider the type in Subfigure 5.1(b). It was already shown that the bound takes into account (i) and (ii) of Proposition 5.7. Following these two rules there are three possible types of flow directions:



The blue arcs are the decisions made. The out-degree w.r.t. the gas flow at the entry node can be 3, 2, or 1. In the leftmost graphic, where $\text{deg}_{\text{gas}}^{\text{out}}(r) = 3$, there has to be at least one arc incident to the exit node on the right along that the gas flows towards the exit node. The arc chosen for this is depicted in blue. Then the

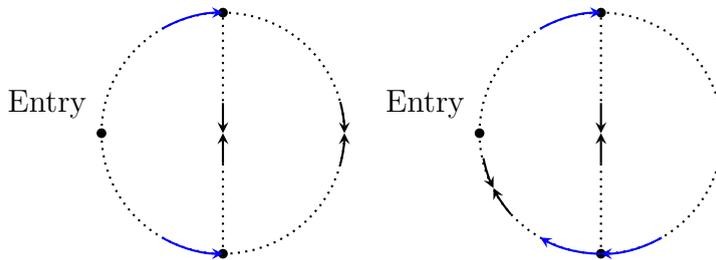
flow along the other two arcs incident to the exit node can be directed towards the exit node or away from it.

In the graphic in the middle, where $\deg_{\text{gas}}^{\text{out}}(r) = 2$, the flow along all of the arcs in the lower bow have to be directed towards the entry node, because the in-degree of every (exit) node in this bow has to be at least 1. Moreover, there has to be at least one arc incident to the exit node on the right along that the gas flows towards the exit node. Again, the arc chosen for this is drawn in blue. Hence, the flow along each arc in the upper bow has to be directed towards the exit node, because the in-degree of every (exit) node in this bow has to be at least 1. Then the flow along the remaining arc incident to the exit node can be directed towards the exit node or away from it.

Finally, in the rightmost graphic the flow along each arc can be fixed from bottom to top.

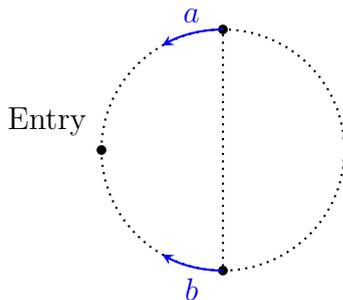
From that it can be seen that every node is served in a network of the type in Subfigure 5.1(b) if rules (i) and (ii) of Proposition 5.7 are met.

Now, consider the type in Subfigure 5.1(a). First, it is shown that every node is served if the gas flow reaches the second cycle. There are two different types of flow directions fulfilling (i) and (ii) of Proposition 5.7 where the gas flow reaches the second cycle. Again, the arcs where a decision was made are depicted in blue.



Hence, every exit node is served.

From this it follows that the only possibility that the gas flow does not serve every exit node is that the gas flow does not reach the second cycle.



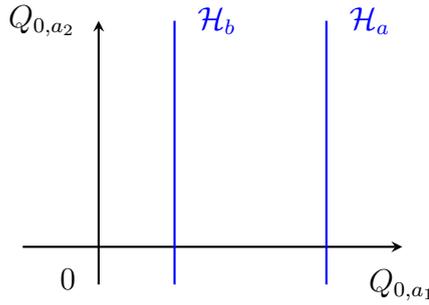
The hyperplanes corresponding to arcs a and b are

$$\mathcal{H}_a = \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : \sum_{u \in D_{\mathcal{T}}(\text{head}(a))} q_u^{\text{nom}} - Q_{0,a_1} = 0 \right\}$$

and

$$\mathcal{H}_b = \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : \sum_{u \in D_{\mathcal{T}}(\text{head}(b))} q_u^{\text{nom}} - Q_{0,a_1} = 0 \right\}$$

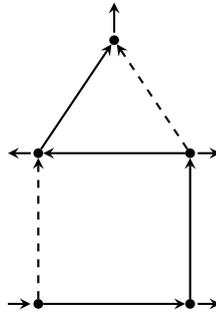
where $D_{\mathcal{T}}(\text{head}(a)) \supset D_{\mathcal{T}}(\text{head}(b))$ and thus, $\sum_{u \in D_{\mathcal{T}}(\text{head}(a))} q_u^{\text{nom}} > \sum_{u \in D_{\mathcal{T}}(\text{head}(b))} q_u^{\text{nom}}$. The two hyperplanes are shown in the following graphic.



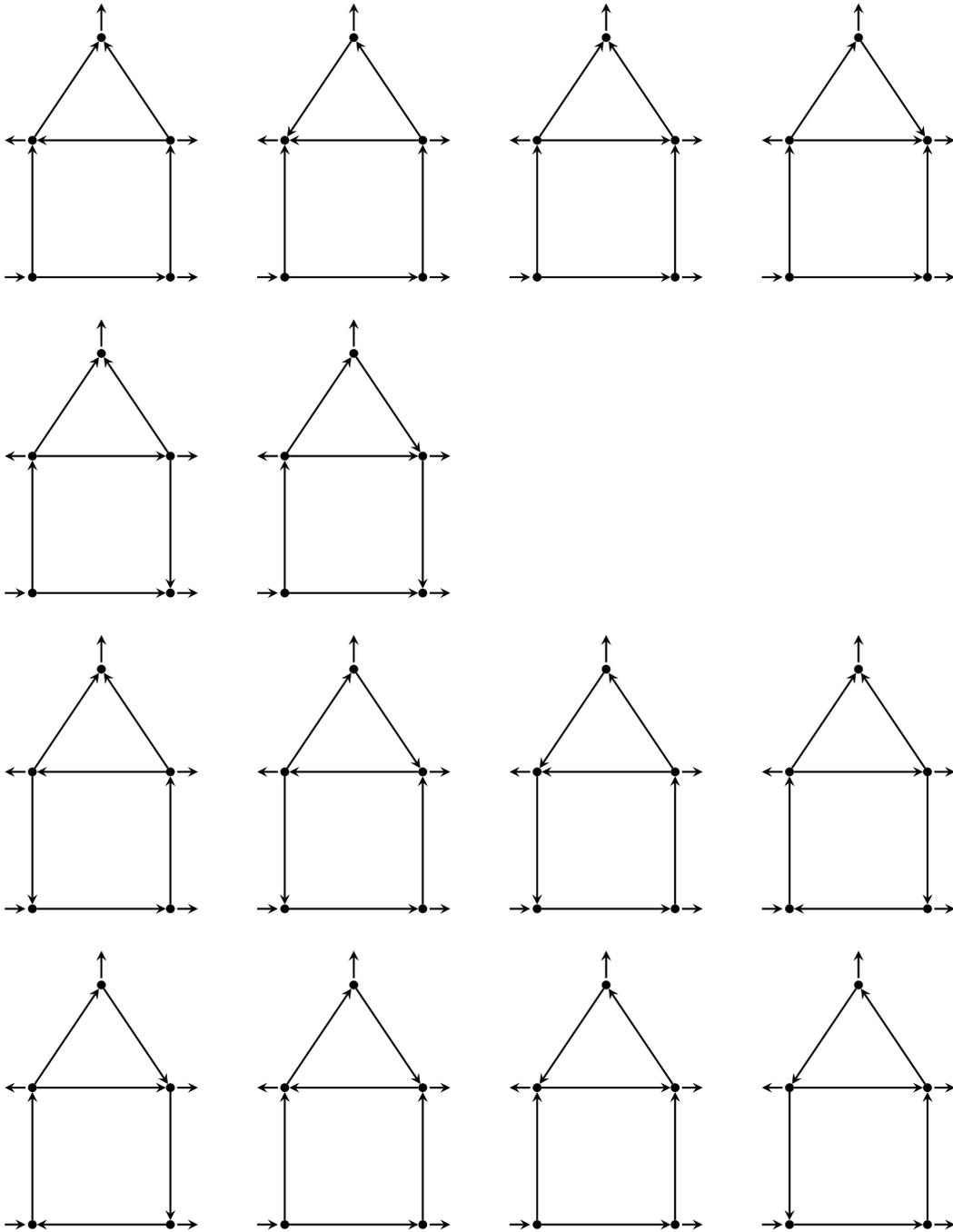
If the flow along arcs a and b is directed in the way shown in the graphic, $Q_{0,a} < 0$ and $Q_{0,b} > 0$ have to hold. But this means that $(Q_{0,a_1}, Q_{0,a_2})^T$ has to be a point right of hyperplane \mathcal{H}_a and left of hyperplane \mathcal{H}_b . Obviously, this is not possible and it can be concluded, that the bound takes into account that every exit node needs to be served. \square

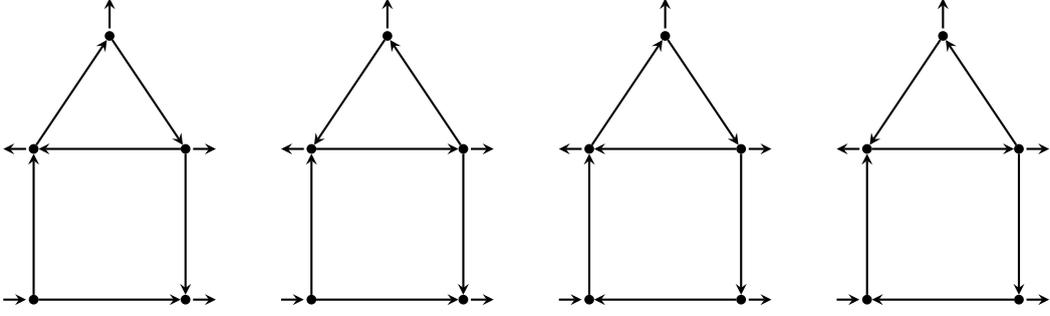
The following example shows that the upper bound of feasible flow directions given in Theorem 5.14 indeed is an upper bound and not exact, because it does not take into account that there cannot be cycles that are directed w.r.t. the gas flow and that the in-degree w.r.t. the gas flow of the reference node r has to be zero.

Example 5.15. Consider the following network with one entry node and four exit nodes consisting of exactly two fundamental cycles that are not edge-disjoint and containing no arcs that do not belong to any cycle.



The network has 6 arcs, thus there are $2^6 = 64$ possible flow directions. By Theorem 5.14 at most 18 of them are feasible due to the rules in Proposition 5.7. These 18 flow directions following (i) and (ii) of Proposition 5.7 and taking into account that every exit node needs to be served are depicted below.





The flow directions depicted in the first two rows follow all of the rules in Proposition 5.7 while the flow directions depicted in the last three rows violate (iv) or (vi) of Proposition 5.7.

The remaining flow directions violating (i) or (ii) of Proposition 5.7 or failing to serve all exit nodes are shown in Figure A.2 in Appendix A.2.

Corollary 5.16. *Let G be a graph representing a network consisting of exactly two fundamental cycles that are not edge-disjoint and containing no arcs that do not belong to any cycle, \mathcal{T} a DFS-tree rooted in the reference node r oriented w.r.t. the predecessor function, \vec{G} the orientation of G w.r.t the spanning tree \mathcal{T} , and $A(\vec{\mathcal{T}}) = \{a_1, a_2\}$. Let r be the only entry node in \vec{G} and assume $q_u^{\text{nom}} > 0$ for all exit nodes $u \in V_-$. Moreover, set $G' = (V', A')$ with*

$$V' := V(G) \setminus \{u \in V_0(G) : \deg(u) = 2\},$$

$$A' := \left\{ \{\text{head}(a), \text{tail}(a)\} : a \in A(\vec{G}) \text{ such that } \text{head}(a) \notin V_0(G) \wedge \text{tail}(a) \notin V_0(G) \right\} \\ \cup \left\{ \{u, v\} : u, v \in V' \wedge \exists \text{ a path } u, b_1, w_1, b_2, w_2, \dots, v \text{ in } G \text{ such that } \right. \\ \left. w_i \in V_0(G) \wedge \deg(w_i) = 2 \forall i \right\}$$

and let \mathcal{T}' be a DFS-tree of G' rooted in node r oriented w.r.t. the predecessor function, \vec{G}' the orientation of G' w.r.t the spanning tree \mathcal{T}' , and $A(\vec{\mathcal{T}}') = \{a'_1, a'_2\}$. Set $\mathcal{P} := \{\mathcal{P}_1, \mathcal{P}_2, \mathcal{P}_3\} = \left\{ \{\mathcal{C}_{a'_1}\}, \{\mathcal{C}_{a'_2}\}, \{\mathcal{C}_{a'_1}, \mathcal{C}_{a'_2}\} \right\}$ (w.r.t. G'). Then there are at most

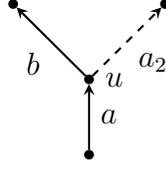
$$\sum_{i=2}^3 \left(|A_{\mathcal{P}_i}| \sum_{j=1}^{i-1} |A_{\mathcal{P}_j}| \right) + |A'| + 1 - |\{u \in V_0(G) : \deg(u) = 3\}| \quad (5.15)$$

feasible flow directions of the gas along the arcs in \vec{G} .

Proof. If \vec{G} does not contain an innode $u \in V_0$ with $\deg(u) = 3$ the number of feasible flow directions of the gas along the arcs in \vec{G} and \vec{G}' are the same by (iii) of Proposition 5.7.

Now let u be an innode of \vec{G} with $\deg(u) = 3$. By Figure 5.1 there are two possible situations.

First, consider the case



where arc a is an arc in cycle \mathcal{C}_{a_1} and arc b an arc in cycles \mathcal{C}_{a_1} and \mathcal{C}_{a_2} . The hyperplanes corresponding to the three arcs are

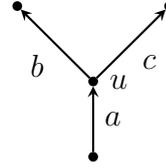
$$\begin{aligned}\mathcal{H}_a &= \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : \sum_{u \in D_{\mathcal{T}}(\text{head}(a))} q_u^{\text{nom}} - Q_{0,a_1} = 0 \right\}, \\ \mathcal{H}_b &= \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : \sum_{u \in D_{\mathcal{T}}(\text{head}(b))} q_u^{\text{nom}} - Q_{0,a_1} - Q_{0,a_2} = 0 \right\}, \\ \mathcal{H}_{a_2} &= \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : Q_{0,a_2} = 0 \right\}\end{aligned}$$

with

$$\sum_{u \in D_{\mathcal{T}}(\text{head}(a))} q_u^{\text{nom}} = \sum_{u \in D_{\mathcal{T}}(\text{head}(b))} q_u^{\text{nom}}.$$

Hence, all three hyperplanes intersect in the point $(\sum_{u \in D_{\mathcal{T}}(\text{head}(a))} q_u^{\text{nom}}, 0)^T$.

In the case



where arc a is an arc in cycles \mathcal{C}_{a_1} and \mathcal{C}_{a_2} , arc b an arc in cycle \mathcal{C}_{a_1} and arc c is an arc in cycle \mathcal{C}_{a_2} , the hyperplanes corresponding to the three arcs are

$$\begin{aligned}\mathcal{H}_a &= \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : \sum_{u \in D_{\mathcal{T}}(\text{head}(a))} q_u^{\text{nom}} - Q_{0,a_1} - Q_{0,a_2} = 0 \right\}, \\ \mathcal{H}_b &= \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : \sum_{u \in D_{\mathcal{T}}(\text{head}(b))} q_u^{\text{nom}} - Q_{0,a_1} = 0 \right\}, \\ \mathcal{H}_c &= \left\{ (Q_{0,a_1}, Q_{0,a_2})^T : \sum_{u \in D_{\mathcal{T}}(\text{head}(c))} q_u^{\text{nom}} - Q_{0,a_2} = 0 \right\}\end{aligned}$$

with

$$\sum_{u \in D_{\mathcal{T}}(\text{head}(a))} q_u^{\text{nom}} = \sum_{u \in D_{\mathcal{T}}(\text{head}(b))} q_u^{\text{nom}} + \sum_{u \in D_{\mathcal{T}}(\text{head}(c))} q_u^{\text{nom}}.$$

Hence, all three hyperplanes intersect in $(\sum_{u \in D_{\mathcal{T}}(\text{head}(b))} q_u^{\text{nom}}, \sum_{u \in D_{\mathcal{T}}(\text{head}(c))} q_u^{\text{nom}})^T$.

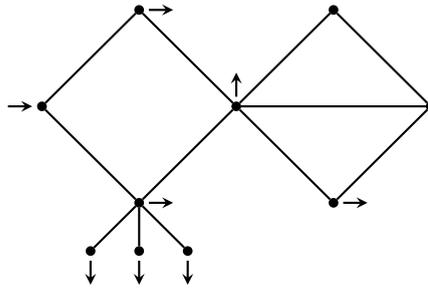
Since the formula of Theorem 5.14 assumes that there are no points where more than two hyperplanes intersect and since the number of areas generated by three

hyperplanes that do not intersect in one point is the number of areas generated by three hyperplanes that do intersect in one point plus 1, the assertion of the lemma holds. \square

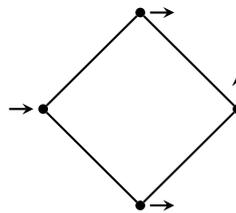
5.2.1.2 General Networks

Corollary 5.17. *Let G be a graph representing a network containing exactly one entry node and assume $q_u^{\text{nom}} > 0$ for all exit nodes $u \in V_-$. Let $G' = (V(G), A')$ where $A' = \{a \in A(G) : \exists C \in \mathcal{C} \text{ with } a \in A(C)\}$. If a component of G' contains cycles that are connected by a node but are pairwise edge-disjoint, the component can be split at this node. The entry nodes and exit nodes of the components obtained in this way are determined in the same way as in (vi) of Proposition 5.7. Then the product of the upper bounds for the number of feasible flow directions of the components of G' is an upper bound for the number of feasible flow directions of G .*

Example 5.18. Consider the following graph.

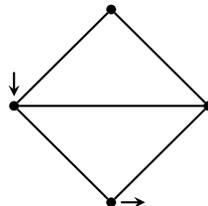


After deletion of the arcs that are not contained in any cycle, the graph decomposes into two components. The first component is

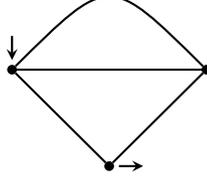


Its upper bound for the number of feasible flow directions is 3 due to Theorem 5.10.

The second component is



By Corollary 5.16 the two arcs at the top can be replaced by one single arc yielding



The upper bound for the number of feasible flow directions of this component is 9 due to Corollary 5.16.

Altogether, this implies that $3 \cdot 9 = 27$ is an upper bound for the number of feasible flow directions. For comparison, without applying Proposition 5.7 there are $2^{12} = 4,096$ possibilities to direct the flow along the arcs.

5.3 Redundant Pressure Bounds

Another possibility to reduce the complexity of system (5.1) – (5.4) are redundant pressure bounds. Elimination of redundant pressure bounds leads to a reduction in the number of terms that have to be considered in the minima and maxima in equations (5.2) – (5.4).

Proposition 5.19. *Let G be a graph representing a given network, \mathcal{T} a DFS-tree rooted in the reference node r oriented w.r.t. the predecessor function, \vec{G} the orientation of G w.r.t. the spanning tree \mathcal{T} , and Q_0 a flow on \vec{G} with corresponding pressure p^+ fulfilling (4.11) and (4.12). Let u and v be two nodes in $V(G)$. Since G is connected, there exists at least one path in G connecting u and v . Let the flow along this path be directed from u to v .*

If the upper pressure bound \bar{p}_u at node u is not greater than the upper pressure bound \bar{p}_v at node v , then \bar{p}_v is redundant and in the minima in equations (5.2) and (5.3), the term $(\bar{p}_v)^2 + g_v(q^{\text{nom}}, z)$ does not have to be considered.

If the lower pressure bound \underline{p}_u at node u is not greater than the lower pressure bound \underline{p}_v at node v , then \underline{p}_u is redundant and in the maxima in equations (5.2) and (5.4), the term $(\underline{p}_u)^2 + g_u(q^{\text{nom}}, z)$ does not have to be considered.

Proof. Assume $\bar{p}_u \leq \bar{p}_v$. Since the gas loses pressure when it flows from node u to node v , $p_u \geq p_v$ holds. Together with this, $p_u \leq \bar{p}_u$ implies $p_v \leq \bar{p}_v$ and redundancy of \bar{p}_v is proven.

Next it has to be shown that

$$(\bar{p}_v)^2 + g_v(q^{\text{nom}}, z) \geq (\bar{p}_u)^2 + g_u(q^{\text{nom}}, z)$$

holds. By equation (5.5) and since $p_w \geq 0$ for all $w \in V$, $p_u \geq p_v$ implies

$$0 \geq (p_v)^2 - (p_u)^2 = g_u(q^{\text{nom}}, z) - g_v(q^{\text{nom}}, z).$$

Together with $\bar{p}_u \leq \bar{p}_v$ this implies

$$(\bar{p}_v)^2 - (\bar{p}_u)^2 \geq 0 \geq g_u(q^{\text{nom}}, z) - g_v(q^{\text{nom}}, z)$$

and thus

$$(\bar{p}_v)^2 + g_v(q^{\text{nom}}, z) \geq (\bar{p}_u)^2 + g_u(q^{\text{nom}}, z)$$

is valid.

The redundancy of \underline{p}_u if $\underline{p}_u \leq \underline{p}_v$ follows analogously. \square

The effect of Proposition 5.19 will become even more meaningful when the probability of exit loads to be feasible is considered. This will be discussed in the next chapter.

Chapter 6

Probability of Feasibility

This chapter deals with the probability of load vectors to be feasible. Section 6.1 gives the theory while Section 6.2 provides some numerical results.

6.1 Computing the Probability of Feasibility Using Spheric-Radial Decomposition

The main ambition of this thesis is to determine the probability of load vectors to be feasible. The loads at entry nodes do not underly any specific distribution because they are driven by prices. Because of that the networks considered in this chapter are restricted to networks with exactly one entry node. In contrast, the exit loads mainly depend on the weather and thus can be identified by a random vector $\xi(\omega)$ on a probability space $(\Omega, \mathbb{A}, \mathbb{P})$ following a multivariate Gaussian distribution with mean vector μ and positive definite covariance matrix Σ , $\xi \sim \mathcal{N}(\mu, \Sigma)$.

Since only networks with exactly one entry node are considered, the definition of the set

$$M_- := \left\{ q_-^{\text{nom}} \in \mathbb{R}^{|V^-|} : \exists \hat{q}^{\text{nom}+} \in \mathbb{R}^{|V^+|} \text{ with } \hat{q}_-^{\text{nom}+} = q_-^{\text{nom}} \text{ s.t. } \hat{q}^{\text{nom}+} \in M \right\}$$

of feasible exit load vectors appears naturally. Hence, one is interested in the probability

$$\mathbb{P}\{\omega \in \Omega : \xi(\omega) \in M_-\}.$$

Such probabilities can be computed with a reparametrization method called spheric-radial decomposition that is known to have better convergence properties than a pure Monte Carlo approach, see, e.g., [33, 50, 51].

Theorem 6.1 (Spheric-Radial Decomposition). *Let $\xi \sim \mathcal{N}(0, R)$ be some n -dimensional standard Gaussian distribution with zero mean and positive definite correlation matrix R . Then, for any Borel measurable subset $\mathcal{R} \subseteq \mathbb{R}^n$ it holds that*

$$\mathbb{P}(\xi \in \mathcal{R}) = \int_{\mathbb{S}^{n-1}} \mu_{\mathcal{X}}\{r \geq 0 : rLv \in \mathcal{R}\} d\mu_{\eta}(v),$$

where \mathbb{S}^{n-1} is the $(n-1)$ -dimensional unit sphere in \mathbb{R}^n , μ_η is the uniform distribution on \mathbb{S}^{n-1} , μ_χ denotes the χ -distribution with n degrees of freedom and L is such that $R = LL^T$ (e.g., Cholesky decomposition).

In contrast to pure Monte Carlo methods the approach following the spheric-radial decomposition does not sample on the full euclidean space \mathbb{R}^n , but only on the unit sphere around the origin. Then the rays starting in the origin and having the direction Lv where v is the sample on the sphere are considered and the intersections of such rays and the set \mathcal{R} are determined. The idea of spheric-radial decomposition is illustrated in Figure 6.1.

If \mathcal{U} is a finite union of disjoint intervals $[a_1, b_1], \dots, [a_k, b_k]$, then $\mu_\chi(\mathcal{U}) = \sum_{i=1}^k (F_\chi(b_i) - F_\chi(a_i))$ where F_χ is the distribution function of μ_χ .

Theorem 6.1 is adaptable to general Gaussian distributions $\xi \sim \mathcal{N}(\mu, \Sigma)$. Let $D := \text{diag}(\sqrt{\Sigma_{ii}})_{i=1, \dots, n}$, then $R := D^{-1}\Sigma D^{-1}$ is the correlation matrix of the distribution.

Let $X \sim \mathcal{N}(\tilde{\mu}, \tilde{\Sigma})$ be a n -dimensional random variable and $Y := BX + c$ for a $n \times n$ matrix B and a n -dimensional vector c . It is a well known fact in probability theory that $Y \sim \mathcal{N}(B\tilde{\mu} + c, B\tilde{\Sigma}B^T)$, cf. [9, 67, 70]. With that it is clear that $\xi^* := D^{-1}(\xi - \mu) \sim \mathcal{N}(0, R)$ is valid.

Moreover, let L be a matrix with $\Sigma = LL^T$, then $R = D^{-1}L(D^{-1}L)^T$ holds.

Putting all this together, one gets

$$\begin{aligned} \mathbb{P}(\xi \in \mathcal{R}) &= \mathbb{P}(\xi^* \in D^{-1}(\mathcal{R} - \mu)) \\ &= \int_{\mathbb{S}^{n-1}} \mu_\chi \{r \geq 0 : rD^{-1}Lv \in D^{-1}(\mathcal{R} - \mu)\} d\mu_\eta(v) \\ &= \int_{\mathbb{S}^{n-1}} \mu_\chi \{r \geq 0 : rLv + \mu \in \mathcal{R}\} d\mu_\eta(v) \end{aligned}$$

by Theorem 6.1.

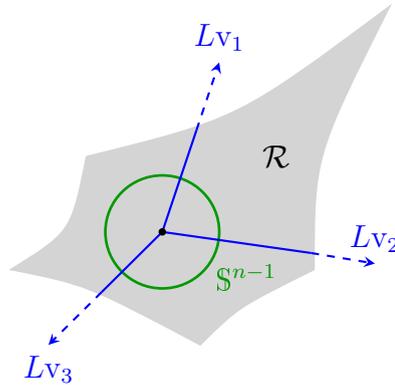


Figure 6.1: Spheric-Radial Decomposition. The set \mathcal{R} of which the probability has to be computed is depicted in gray. The green circle represents the unit sphere. Three directions sampled on the sphere are drawn in blue. Only the solid line segments are relevant for the computation of the probability.

The following algorithm for the computation of the probability of feasible exit loads arises.

Algorithm 6.2 (Probability of Feasible Exit Load Vectors).

Input: A gas network, a random variable ξ representing the exit load vector,
 $\xi \sim \mathcal{N}(\mu, \Sigma)$, L such that $LL^T = \Sigma$, number of samples d .

Output: Probability of feasible exit load vectors

$\mathcal{S} :=$ set of d samples uniformly distributed on the sphere $\mathbb{S}^{|V|-1}$

FOR $v \in \mathcal{S}$ DO

 Compute the one-dimensional set $M_-(v) := \{r \geq 0 : rLv + \mu \in M_-\}$

RETURN $\mathbb{P}(\xi \in M_-) \approx d^{-1} \sum_{v \in \mathcal{S}} \mu_\chi(M_-(v))$

The same approach was already utilized in [57]. But there only networks with at most one cycle were considered. The research in this thesis goes a step further. In the following it is illustrated how networks with several fundamental cycles that are not edge-disjoint are tackled.

The most intricate part of this algorithm is the determination of the sets $M_-(v)$. With $q^{\text{nom}}(r) := rLv + \mu$ the characterization of feasible loads in Theorem 5.1 implies that $M_-(v)$ consists of all $r \in \mathbb{R}_{\geq 0}$ for which there is a z such that

$$\begin{aligned} \mathcal{A}_N^T g(rLv + \mu, z) &= \Phi_N |z| z \\ \min_{i=1, \dots, |V|} [(\bar{p}_{u_i})^2 + g_i(rLv + \mu, z)] &\geq \max_{i=1, \dots, |V|} [(p_{u_i})^2 + g_i(rLv + \mu, z)] \\ (p_{u_0})^2 &\leq \min_{i=1, \dots, |V|} [(\bar{p}_{u_i})^2 + g_i(rLv + \mu, z)] \\ (\bar{p}_{u_0})^2 &\geq \max_{i=1, \dots, |V|} [(p_{u_i})^2 + g_i(rLv + \mu, z)]. \end{aligned}$$

Instead of the minima and maxima, every term can be compared separately yielding the system

$$\begin{aligned} \mathcal{A}_N^T g(rLv + \mu, z) &= \Phi_N |z| z \\ (\bar{p}_{u_i})^2 + g_i(rLv + \mu, z) &\geq (p_{u_j})^2 + g_j(rLv + \mu, z) \quad \text{for all } i, j = 1, \dots, \\ &|V|, i \neq j \quad (6.1) \\ (p_{u_0})^2 &\leq (\bar{p}_{u_i})^2 + g_i(rLv + \mu, z) \quad \text{for all } i = 1, \dots, |V| \\ (\bar{p}_{u_0})^2 &\geq (p_{u_i})^2 + g_i(rLv + \mu, z) \quad \text{for all } i = 1, \dots, |V|. \end{aligned}$$

In order to rewrite the inequalities as a single one, a map $\mathcal{D}: \mathbb{R} \times \mathbb{R}^{|\mathcal{A}(\bar{T})|} \rightarrow |V|(|V| - 1) + 2|V|$ is defined. The components of \mathcal{D} corresponding to the three different types of inequalities are given separately.

- $k = 1, \dots, |V|(|V| - 1)$:

for $i = 1, \dots, |V|$ set

$$k := \begin{cases} (i-1)|V| - i + j + 1 & \text{for } j = 1, \dots, i-1 \\ (i-1)|V| - i + j & \text{for } j = i+1, \dots, |V| \end{cases}$$

and

$$\mathcal{D}_k(\mathbf{r}, z) := (\underline{p}_{u_j})^2 + g_j(\mathbf{r}L\mathbf{v} + \mu, z) - (\bar{p}_{u_i})^2 - g_i(\mathbf{r}L\mathbf{v} + \mu, z)$$

- $k = |V|(|V| - 1) + 1, \dots, |V|(|V| - 1) + |V|$:

for $i = 1, \dots, |V|$ set

$$k := |V|(|V| - 1) + i$$

and

$$\mathcal{D}_k(\mathbf{r}, z) := (\underline{p}_{u_0})^2 - (\bar{p}_{u_i})^2 - g_i(\mathbf{r}L\mathbf{v} + \mu, z)$$

- $k = |V|(|V| - 1) + |V| + 1, \dots, |V|(|V| - 1) + 2|V|$:

for $i = 1, \dots, |V|$ set

$$k := |V|(|V| - 1) + |V| + i$$

and

$$\mathcal{D}_k(\mathbf{r}, z) := (\underline{p}_{u_i})^2 + g_i(\mathbf{r}L\mathbf{v} + \mu, z) - (\bar{p}_{u_0})^2.$$

With this notation system (6.1) can be expressed in the form

$$\begin{aligned} \mathcal{A}_N^T g(\mathbf{r}L\mathbf{v} + \mu, z) &= \Phi_N |z| z \\ \mathcal{D}(\mathbf{r}, z) &\leq 0. \end{aligned} \tag{6.2}$$

By Theorems 5.5 and 5.6, the set M_- of feasible exit load vectors is bounded and closed. Therefore, $M_-(\mathbf{v})$ can be represented as a finite union of disjoint closed intervals. This means that it is sufficient to determine the end points of these subintervals, i.e., to determine the points where the ray enters and exits the set M_- of feasible exit load vectors. In these points one of the inequalities in system (6.2) has to hold with equality. Hence, to determine the end points of all of the subintervals of $M_-(\mathbf{v})$ the system

$$\begin{aligned} \mathcal{A}_N^T g(\mathbf{r}L\mathbf{v} + \mu, z) &= \Phi_N |z| z \\ \mathcal{D}_j(\mathbf{r}, z) &= 0 \\ \mathcal{D}_k(\mathbf{r}, z) &\leq 0 \quad \forall k = 1, \dots, |V|(|V| - 1) + 2|V|, k \neq j \end{aligned}$$

has to be solved for each $j = 1, \dots, |V|(|V| - 1) + 2|V|$.

Here, redundant pressure bounds play an even more important role than in the characterization in Theorem 5.1, because in this setting they reduce the number

of systems to be solved considerably. Strictly speaking, one redundant pressure bound leads to the deletion of $|V|$ components of map \mathcal{D} . The dimension of this effect becomes even more outstanding if one takes into account that the number of components of the map \mathcal{D} has to be multiplied by the number of resolvings of absolute values to determine the number of systems to be solved with the Gröbner basis method of Subsection 2.2.5. Some numerical results of this procedure are shown in Table 6.1 in Section 6.2.

The computation of the sets $M_-(\mathbf{v})$ is summarized in Algorithm 6.3. Let $S \subseteq \{-1, 1\}^{|A|}$ be the set of all feasible resolvings of the absolute values after applying Proposition 5.7. For a given arc $a \in A$ the component s_a is $+1$ if the flow along arc a is directed in the same direction as the arc is directed in the spanning tree \mathcal{T} and -1 otherwise. For each $s \in S$ let P_s be the set of all k such that \mathcal{D}_k is nonredundant according to Proposition 5.19.

Algorithm 6.3 (Computation of $M_-(\mathbf{v})$).

Input: Matrices \mathcal{A}^+ and Φ and vectors \underline{p}^+ and \bar{p}^+ representing the network, a reference node r , a mean value μ , a matrix L such that LL^T equals the covariance matrix, a sample \mathbf{v} , set of feasible flow directions S , for each flow direction $s \in S$ the set of nonredundant inequalities P_s

Output: $M_-(\mathbf{v})$

IF μ is a feasible exit load vector DO

$$M_-(\mathbf{v}) := \{0\}$$

ELSE DO

$$M_-(\mathbf{v}) := \emptyset$$

FOR $s \in S$ DO

FOR $k \in P_s$ DO

solutions := set of solutions of

$$\mathcal{A}_N^T (\mathcal{A}_B^{-1})^T \Phi_B \text{diag}(s_B) \left(\mathcal{A}_B^{-1} (rLv + \mu - \mathcal{A}_N z) \right)^2 = \Phi_N \text{diag}(s_N) z^2$$

$$\mathcal{D}_k(r, z) = 0$$

FOR $(\hat{z}, \hat{r}) \in$ solutions DO

$$\text{IF } \hat{r} \geq 0 \text{ AND } \text{diag}(s_B) \left(\mathcal{A}_B^{-1} (rLv + \mu - \mathcal{A}_N \hat{z}) \right) \geq 0 \text{ AND}$$

$$\text{diag}(s_N) \hat{z} \geq 0 \text{ AND } \mathcal{D}_j(\hat{r}, \hat{z}) \leq 0 \text{ for all } j \in P_s \text{ AND } \hat{r} \notin M_-(\mathbf{v})$$

DO

$$M_-(\mathbf{v}) := M_-(\mathbf{v}) \cup \hat{r}$$

sort the elements of $M_-(\mathbf{v})$ by increasing value

RETURN $\bigcup_{j=1}^{|M_-(\mathbf{v})|/2} [M_-(\mathbf{v})_{2j-1}, M_-(\mathbf{v})_{2j}]$

6.2 Computational Results

This chapter provides some numerical results on computing the probability of feasibility.

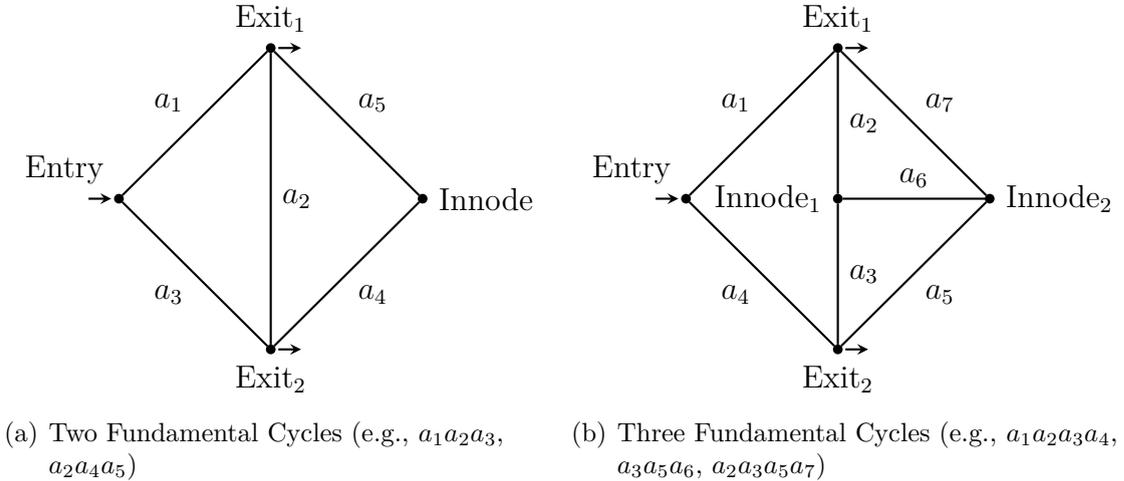


Figure 6.2: Topology of the Networks.

	Original			Reduced		
	Flow Direc.	Nonred. Ineq.	Systems	Flow Direc.	Nonred. Ineq.	Systems
2 Cycles	32	32×12	384	2	2×1	2
3 Cycles	128	128×20	2560	4	$2 \times 1, 2 \times 2$	6

Table 6.1: The number of flow directions, the number of nonredundant inequalities and the number of the polynomial systems to be solved in each sample before and after applying Proposition 5.7 and Proposition 5.19 for the networks with two and three fundamental cycles depicted in Figure 6.2.

To generate the samples, $|V_-|$ -dimensional samples are drawn from the uniform distribution over $[-1, 1]^{|V_-|}$. Then these samples are normalized to unit length and expanded to $|V|$ -dimensional vectors by adding zeros at the positions of the innodes.

All computations are performed by a Python ([96]) implementation on a Windows system equipped with Intel(R) Core(TM) i7 CPU @ 2.60GHz and 8 GB RAM. The polynomial systems are solved by the function `lex_solve` of the library `solve` [92] of the computer algebra system SINGULAR [34].

Figure 6.2 shows the topology of the networks that are considered. The data of these networks is listed in more detail in Appendix B.

Table 6.1 shows the number of flow directions, the number of nonredundant inequalities and the number of the polynomial systems to be solved in each sample before and after applying Proposition 5.7 and Proposition 5.19. It becomes evident that the techniques yield an enormous reduction of the number of systems to be solved in each sample and thus an appreciable reduction of the computing time.

The probability of feasibility is computed for a series of 10 tests with sample

	2 Cycles	3 Cycles
No. of Nodes	4	5
No. of Pipes	5	7
No. of Cycles	2	3
No. of Exits	2	2
No. of Systems per Sample (after reduction)	2	6
Mean Probability	0.94477	0.83290
Variance	6.14014e-6	1.01239e-4
Standard Deviation	0.00248	0.01006
Mean Time	12.22 min	56.32 min

Table 6.2: Summary of dimensions, test results, and computing times for gas networks with two and three fundamental cycles that are not edge-disjoint.

size 1000 each. The results are listed in Table 6.2.

There occur numerical problems in some of the samples, so that these samples could not contribute to the computation of the probability. But the number of these samples is always less than 4.5% of the sample size.

The more fundamental cycles are contained in the network the more time consuming the computation of the solutions of the polynomial systems in SINGULAR becomes, explaining the increase of the computing time. Moreover, in the test case concerning the network with three fundamental cycles there have to be solved three times more polynomial systems per sample than in the test case concerning the network with two fundamental cycles.

Furthermore, Table 6.2 shows that the variance and the standard deviation is sufficiently small.

In Figure 6.3 the moving average of the probability of feasibility with respect to the number of samples is plotted. The probability computed with spheric-radial decomposition is depicted in blue, whereas the probability computed with pure Monte Carlo sampling is drawn in green. It is easily seen that the approach using spheric-radial decomposition converges faster than the approach using pure Monte Carlo sampling. Moreover, Figure 6.3 indicates that far less than 1000 samples are needed to get a meaningful probability when using spheric-radial decomposition.

It has already been mentioned that not all of the systems to be solved during spheric-radial decomposition have a solution and that one advantage of the approach using Gröbner bases in comparison to numerical methods is, that it is much faster in detecting infeasibility of polynomial systems. The average number of systems without solution over the 10 test series is 33.2 for the network with two fundamental cycles depicted in Figure 6.2(a) and 782.2 for the network with three fundamental cycles depicted in Figure 6.2(b). The infeasible polynomial systems occurring during the computations concerning the network with two fundamental

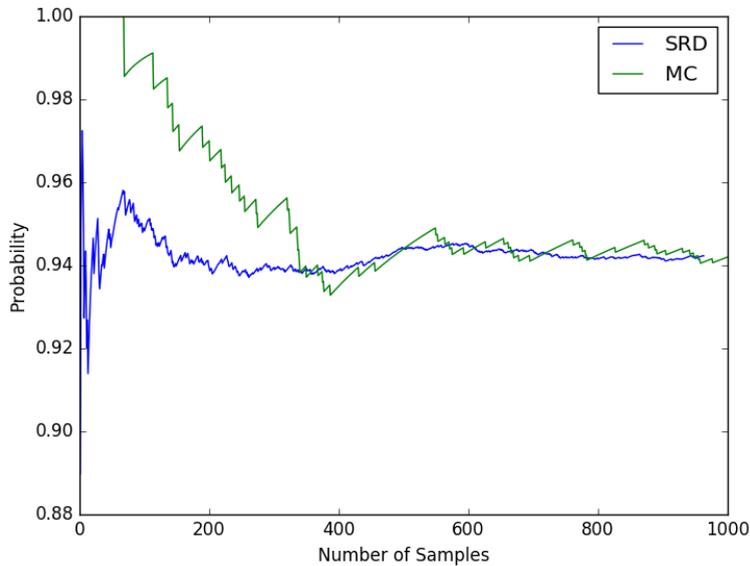


Figure 6.3: Moving average of the probability computed with spheric-radial decomposition (blue) and with pure Monte Carlo sampling (green) with respect to the number of samples for the test network with two fundamental cycles (Figure 6.2(a)).

cycles are “solved” 700 times faster using the function `lex_solve` of SINGULAR than a numerical solver (in Python) needs to detect infeasibility. Taking into account the high number of times this happens, this fact becomes even more crucial.

If networks with more than three fundamental cycles that are not edge-disjoint are considered, the coefficients of the polynomials in the Gröbner basis reach a size with that the polynomial systems become numerically unstable. Hence, too many samples can not be solved and the probabilities computed are unreliable. In [47, 85, 86, 89] the same observation was made when using Gröbner bases for solving the load flow problem of electrical networks.

Chapter 7

Explicit Representation of the Set of Feasible Load Vectors

As already mentioned in the introduction it is an task of high importance for parametric optimization to identify an explicit representation of the set of feasible load vectors. Moreover, it is possible to include this representation into the computation of the probability of feasibility in Chapter 6. However, the required computations are formidable and the representation obtained becomes quite hard to interpret.

To determine an explicit representation of the set of feasible load vectors equation (5.1) has to be solved parametrically with parameter q^{nom} . Afterwards, these solutions can be inserted into the inequalities (5.2) – (5.4) and one gets a system of inequalities that determines the set of feasible load vectors.

To solve equation (5.1) parametrically the absolute values have to be resolved. Again, Proposition 5.7 can be utilized to reduce the number of systems to be considered. For ideals generated by the rows of these polynomial systems in $\mathbb{R}[q^{\text{nom}}][z]$ a disjoint, reduced comprehensive Gröbner system w.r.t. the lexicographic ordering is computed yielding polynomial systems that are much easier to solve. For these computations the library `grobcov` [88] of the computer algebra system SINGULAR [34] can be used. The function `cgsdr` in that library uses the algorithm proposed in [64]. Consider a branch $(\mathbf{V}(E) \setminus \mathbf{V}(N), \mathcal{G})$ of such a comprehensive Gröbner system. The elements of E and N are polynomials in q^{nom} . Hence, with the additional condition that $q_u^{\text{nom}} > 0$ for $u \in V_-$, $q_u^{\text{nom}} < 0$ for $u \in V_+$ and $q_u^{\text{nom}} = 0$ for $u \in V_0$, the set $\mathbf{V}(E) \setminus \mathbf{V}(N)$ can be empty. These branches do not have to be considered any further. Since the lexicographic ordering is used the polynomial system of the branches of the comprehensive Gröbner systems are in triangular form. The univariate polynomial equations of these systems can be solved with the function `solve` of MuPAD in Matlab [82].

The procedure is summarized in the following algorithm. The set of load vectors $q^{\text{nom}+}$ for that q^{nom} and the corresponding z fulfill inequalities (5.2) – (5.4) is denoted $Z(z)$.

Algorithm 7.1.

Input: Matrices \mathcal{A}^+ and Φ and vectors \underline{p}^+ and \bar{p}^+ representing the network, a DFS-tree \mathcal{T} rooted in the reference node, set of feasible flow directions S .

Output: Explicit description of the set of feasible load vectors M

$M := \emptyset$

FOR $s \in S$ DO

$$\mathcal{F} := \mathcal{A}_N^T (\mathcal{A}_B^{-1})^T \Phi_B \text{diag}(s_B) \left(\mathcal{A}_B^{-1} (q^{\text{nom}} - \mathcal{A}_N z) \right)^2 - \Phi_N \text{diag}(s_N) z^2$$

$$\mathcal{I} := \langle \mathcal{F}_1, \dots, \mathcal{F}_{|\mathcal{A}(\bar{\mathcal{T}})|} \rangle \subseteq \mathbb{R}[q^{\text{nom}}][z]$$

$\tilde{\mathcal{G}}$:= disjoint, reduced comprehensive Gröbner system of \mathcal{I} w.r.t. the lexicographic ordering

Delete branches $(\mathbf{V}(E) \setminus \mathbf{V}(N), \mathcal{G})$ from $\tilde{\mathcal{G}}$ with $\mathbf{V}(E) \setminus \mathbf{V}(N) = \emptyset$ (under the condition $q_u^{\text{nom}} > 0$ for $u \in V_-$, $q_u^{\text{nom}} < 0$ for $u \in V_+$ and $q_u^{\text{nom}} = 0$ for $u \in V_0$)

FOR EACH branch $(\mathbf{V}(E) \setminus \mathbf{V}(N), \mathcal{G})$ of $\tilde{\mathcal{G}}$ DO

solutions := set of solutions of the parametric polynomial system of the polynomials in \mathcal{G}

FOR EACH $Q_{0,N}(q^{\text{nom}}) \in$ solutions DO

$$X := \left\{ q^{\text{nom}+} : \begin{aligned} &\text{diag}(s_B) \left(\mathcal{A}_B^{-1} (q^{\text{nom}} - \mathcal{A}_N Q_{0,N}(q^{\text{nom}})) \right) \geq 0 \\ &\wedge \text{diag}(s_N) Q_{0,N}(q^{\text{nom}}) \geq 0 \end{aligned} \right\}$$

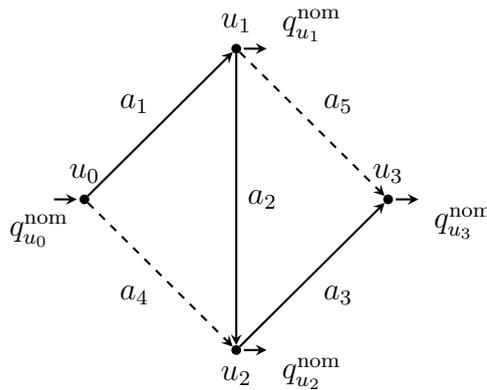
$$M := M \cup \left(X \cap Z(Q_{0,N}(q^{\text{nom}})) \cap (\mathbf{V}(E) \setminus \mathbf{V}(N)) \cap \left\{ q^{\text{nom}+} : \mathbf{1}^T q^{\text{nom}+} = 0 \right\} \right)$$

RETURN M

A drawback of this procedure is that networks with more than two fundamental cycles that are not edge-disjoint cannot be tackled by the computer ¹ used because it runs out of memory.

The procedure is demonstrated on an example.

Example 7.2. Consider the network depicted below.



¹Windows system equipped with Intel(R) Core(TM) i7 CPU @ 2.60GHz and 8GB RAM

To simplify notation and to shorten formulas by reducing the length of coefficients, the pressure drop coefficients of the pipes are assumed to be 1. The set of feasible load vectors then reads

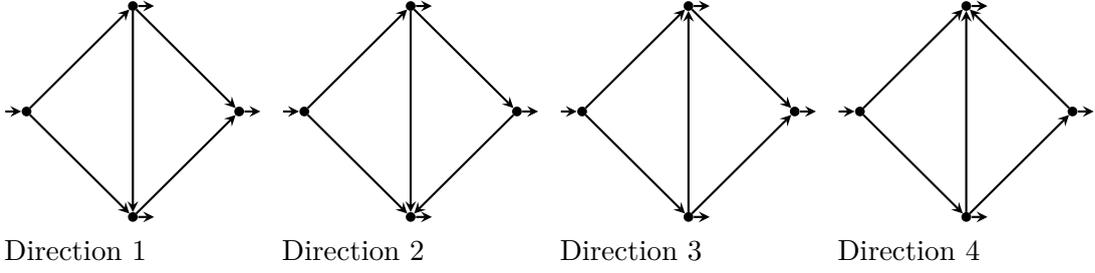
$$M = \{q^{\text{nom}+} : \mathbf{1}^T q^{\text{nom}+} = 0,$$

$\exists z$ such that

$$\begin{aligned} |z_1| z_1 &= |q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1| (q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1) \\ &\quad + |q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2| (q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2) \\ |z_2| z_2 &= |q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2| (q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2) \\ &\quad + |q_{u_3}^{\text{nom}} - z_2| (q_{u_3}^{\text{nom}} - z_2) \\ (\bar{p}_{u_1})^2 &\geq (\underline{p}_{u_2})^2 + |q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2| (q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2) \\ (\bar{p}_{u_1})^2 &\geq (\underline{p}_{u_3})^2 + |q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2| (q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2) \\ &\quad + |q_{u_3}^{\text{nom}} - z_2| (q_{u_3}^{\text{nom}} - z_2) \\ (\bar{p}_{u_2})^2 &\geq (\underline{p}_{u_1})^2 - |q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2| (q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2) \\ (\bar{p}_{u_2})^2 &\geq (\underline{p}_{u_3})^2 + |q_{u_3}^{\text{nom}} - z_2| (q_{u_3}^{\text{nom}} - z_2) \\ (\bar{p}_{u_3})^2 &\geq (\underline{p}_{u_1})^2 - |q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2| (q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2) \\ &\quad - |q_{u_3}^{\text{nom}} - z_2| (q_{u_3}^{\text{nom}} - z_2) \\ (\bar{p}_{u_3})^2 &\geq (\underline{p}_{u_2})^2 - |q_{u_3}^{\text{nom}} - z_2| (q_{u_3}^{\text{nom}} - z_2) \\ (\underline{p}_{u_0})^2 &\leq (\bar{p}_{u_1})^2 + |q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1| (q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1) \\ (\underline{p}_{u_0})^2 &\leq (\bar{p}_{u_2})^2 + |q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1| (q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1) \\ &\quad + |q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2| (q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2) \\ (\underline{p}_{u_0})^2 &\leq (\bar{p}_{u_3})^2 + |q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1| (q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1) \\ &\quad + |q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2| (q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2) \\ &\quad + |q_{u_3}^{\text{nom}} - z_2| (q_{u_3}^{\text{nom}} - z_2) \\ (\bar{p}_{u_0})^2 &\geq (\underline{p}_{u_1})^2 + |q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1| (q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1) \\ (\bar{p}_{u_0})^2 &\geq (\underline{p}_{u_2})^2 + |q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1| (q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1) \\ &\quad + |q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2| (q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2) \\ (\bar{p}_{u_0})^2 &\geq (\underline{p}_{u_2})^2 + |q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1| (q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1) \\ &\quad + |q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2| (q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2) \\ &\quad + |q_{u_3}^{\text{nom}} - z_2| (q_{u_3}^{\text{nom}} - z_2) \} \end{aligned}$$

by Theorem 5.1. The set of load vectors $q^{\text{nom}+}$ for that q^{nom} and corresponding (z_1, z_2) fulfill the inequalities in above description is denoted $Z(z_1, z_2)$.

The network contains exactly one entry node, u_0 , this means that the flow along arcs a_1 and a_4 has to be directed away from node u_0 by (vi) of Proposition 5.7. The feasible flow directions along arcs a_2 , a_3 and a_5 are shown below while the infeasible flow directions are listed in Figure A.3 in Appendix A.3.



Now, the different flow directions are considered separately. The first direction is discussed in more detail, but for the remaining directions only the results are listed. The superscripts in brackets indicate the flow direction to which the formulas belong.

Direction 1: $Q_{0,a_1} = q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4} \geq 0$, $Q_{0,a_2} = q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4} - Q_{0,a_5} \geq 0$, $Q_{0,a_3} = q_{u_3}^{\text{nom}} - Q_{0,a_5} \geq 0$, $Q_{0,a_4} = z_1 \geq 0$, $Q_{0,a_5} = z_2 \geq 0$

Pressure drop polynomials:

$$h_1^{(1)} = \left(q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 \right)^2 + \left(q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2 \right)^2 - z_1^2$$

$$h_2^{(1)} = \left(q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2 \right)^2 + \left(q_{u_3}^{\text{nom}} - z_2 \right)^2 - z_2^2$$

Comprehensive Gröbner system of $\langle h_1^{(1)}, h_2^{(1)} \rangle \subseteq \mathbb{R}[q_{u_1}^{\text{nom}}, q_{u_2}^{\text{nom}}, q_{u_3}^{\text{nom}}][z_1, z_2]$:

IF $\left(q_{u_1}^{\text{nom}} \right)^2 + 2q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} + 3q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} + \left(q_{u_2}^{\text{nom}} \right)^2 + 3q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + 2\left(q_{u_3}^{\text{nom}} \right)^2 \neq 0$:

$$g_1^{(1)} = \left(4\left(q_{u_1}^{\text{nom}} \right)^2 + 8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} + 16q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} + 4\left(q_{u_2}^{\text{nom}} \right)^2 + 16q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + 16\left(q_{u_3}^{\text{nom}} \right)^2 \right) z_2^2$$

$$+ \left(4\left(q_{u_1}^{\text{nom}} \right)^3 + 4\left(q_{u_1}^{\text{nom}} \right)^2q_{u_2}^{\text{nom}} - 4q_{u_1}^{\text{nom}}\left(q_{u_2}^{\text{nom}} \right)^2 - 24q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} \right.$$

$$\left. - 24q_{u_1}^{\text{nom}}\left(q_{u_3}^{\text{nom}} \right)^2 - 4\left(q_{u_2}^{\text{nom}} \right)^3 - 24\left(q_{u_2}^{\text{nom}} \right)^2q_{u_3}^{\text{nom}} - 40q_{u_2}^{\text{nom}}\left(q_{u_3}^{\text{nom}} \right)^2 - 24\left(q_{u_3}^{\text{nom}} \right)^3 \right) z_2$$

$$+ \left(q_{u_1}^{\text{nom}} \right)^4 - 2\left(q_{u_1}^{\text{nom}} \right)^2\left(q_{u_2}^{\text{nom}} \right)^2 - 4\left(q_{u_1}^{\text{nom}} \right)^2q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + 8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}}\left(q_{u_3}^{\text{nom}} \right)^2$$

$$+ 8q_{u_1}^{\text{nom}}\left(q_{u_3}^{\text{nom}} \right)^3 + \left(q_{u_2}^{\text{nom}} \right)^4 + 4\left(q_{u_2}^{\text{nom}} \right)^3q_{u_3}^{\text{nom}} + 12\left(q_{u_2}^{\text{nom}} \right)^2\left(q_{u_3}^{\text{nom}} \right)^2$$

$$+ 16q_{u_2}^{\text{nom}}\left(q_{u_3}^{\text{nom}} \right)^3 + 8\left(q_{u_3}^{\text{nom}} \right)^4$$

$$g_2^{(1)} = \left(2q_{u_1}^{\text{nom}} + 2q_{u_2}^{\text{nom}} + 2q_{u_3}^{\text{nom}} \right) z_1 - 2q_{u_3}^{\text{nom}}z_2 - \left(q_{u_1}^{\text{nom}} \right)^2 - 2q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} - 2q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}}$$

$$- \left(q_{u_2}^{\text{nom}} \right)^2 - 2q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}}$$

IF $q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + 2q_{u_3}^{\text{nom}} = 0$ AND $q_{u_3}^{\text{nom}} \neq 0$:

$$g_1^{(1)} = 2\left(q_{u_3}^{\text{nom}} \right)^2 z_2 - \left(q_{u_2}^{\text{nom}} \right)^2 q_{u_3}^{\text{nom}} - 2q_{u_2}^{\text{nom}}\left(q_{u_3}^{\text{nom}} \right)^2 - 2\left(q_{u_3}^{\text{nom}} \right)^3$$

$$g_2^{(1)} = q_{u_3}^{\text{nom}}z_1 + q_{u_3}^{\text{nom}}z_2$$

IF $q_{u_3}^{\text{nom}} = 0$ AND $q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} = 0$:

$$g_1^{(1)} = z_1^2 + 2z_1z_2 - 2q_{u_2}^{\text{nom}}z_1 + z_2^2 - 2q_{u_2}^{\text{nom}}z_2 + (q_{u_2}^{\text{nom}})^2$$

IF $q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} = 0$ AND $q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} + q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + 2(q_{u_3}^{\text{nom}})^2 \neq 0$:

$$g_1^{(1)} = 2q_{u_3}^{\text{nom}}z_2 - (q_{u_3}^{\text{nom}})^2$$

$$g_2^{(1)} = z_1^2 + 2z_1z_2 + (-2q_{u_2}^{\text{nom}} - 2q_{u_3}^{\text{nom}})z_1 + z_2^2 + (-2q_{u_2}^{\text{nom}})z_2 + (q_{u_2}^{\text{nom}})^2 + 2q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}}$$

Since nodes u_1 , u_2 and u_3 are exit nodes, $q_1^{\text{nom}}, q_2^{\text{nom}}, q_3^{\text{nom}} \geq 0$ holds. Thus, the condition $(q_{u_1}^{\text{nom}})^2 + 2q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} + 3q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} + (q_{u_2}^{\text{nom}})^2 + 3q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + 2(q_{u_3}^{\text{nom}})^2 = 0$, the only way not to be in the first branch, is only fulfilled with $q_1^{\text{nom}} = q_2^{\text{nom}} = q_3^{\text{nom}} = 0$. Obviously, this case is irrelevant, because this would mean that there is no gas flow in the network and hence, the first branch is the only relevant branch. In what follows the irrelevant branches will be ignored and for the remaining orientations they will not even be presented here.

Moreover, the basis of the first branch, set-theoretic the biggest one, has the shape mentioned in the Shape Lemma 2.35 while the smaller branches have not.

The two roots of $g_1^{(1)} = 0$, $g_2^{(1)} = 0$ of the first branch are $(Q_{0,a_4}^{(1,i)}(q^{\text{nom}}), Q_{0,a_5}^{(1,i)}(q^{\text{nom}}))$ for $i = 1, 2$ with

$$Q_{0,a_5}^{(1,i)}(q^{\text{nom}}) := \frac{1}{2 \left((q_{u_1}^{\text{nom}})^2 + 2q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} + 4q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} + (q_{u_2}^{\text{nom}})^2 + 4q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + 4(q_{u_3}^{\text{nom}})^2 \right)}$$

$$\left((-1)^i 2\sqrt{q_{u_3}^{\text{nom}}(q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}})^3} \right.$$

$$\left. \sqrt{-(q_{u_1}^{\text{nom}})^2 - q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} + (q_{u_2}^{\text{nom}})^2 + 3q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + (q_{u_3}^{\text{nom}})^2} \right.$$

$$+ q_{u_1}^{\text{nom}}(q_{u_2}^{\text{nom}})^2 - (q_{u_1}^{\text{nom}})^2q_{u_2}^{\text{nom}} + 6q_{u_1}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 + 10q_{u_2}^{\text{nom}}(q_{u_3}^{\text{nom}})^2$$

$$+ 6(q_{u_2}^{\text{nom}})^2q_{u_3}^{\text{nom}} - (q_{u_1}^{\text{nom}})^3 + (q_{u_2}^{\text{nom}})^3 + 6(q_{u_3}^{\text{nom}})^3 + 6q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}})$$

$$Q_{0,a_4}^{(1,i)}(q^{\text{nom}}) := \frac{1}{2(q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}})} \left(2q_{u_3}^{\text{nom}}Q_{0,a_5}^{(1,i)}(q^{\text{nom}}) + (q_{u_1}^{\text{nom}})^2 + 2q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} \right.$$

$$\left. + 2q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} + (q_{u_2}^{\text{nom}})^2 + 2q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} \right).$$

This implies that the set of feasible load vectors that indicate a gas flow according to the first direction is

$$M^{(1)} := \bigcup_{i=1,2} \left(X^{(1,i)} \cap Z^{(1,i)} \right) \cap Y^{(1)} \cap \{q^{\text{nom}+} : \mathbf{1}^T q^{\text{nom}+} = 0\}.$$

Here, $X^{(1,i)}$ contains the inequalities corresponding to the flow direction, $Y^{(1)}$ the

parametric constraints of the branch and $Z^{(1,i)}$ the inequalities in $Z(Q_{0,a_4}^{(1,i)}, Q_{0,a_5}^{(1,i)})$:

$$\begin{aligned} X^{(1,i)} &:= \left\{ q^{\text{nom}+} : q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4}^{(1,i)}(q^{\text{nom}}) \geq 0, q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4}^{(1,i)}(q^{\text{nom}}) \right. \\ &\quad \left. - Q_{0,a_5}^{(1,i)}(q^{\text{nom}}) \geq 0, q_{u_3}^{\text{nom}} - Q_{0,a_5}^{(1,i)}(q^{\text{nom}}) \geq 0, Q_{0,a_4}^{(1,i)}(q^{\text{nom}}) \geq 0, \right. \\ &\quad \left. Q_{0,a_5}^{(1,i)}(q^{\text{nom}}) \geq 0 \right\} \\ Y^{(1)} &:= \left\{ q^{\text{nom}+} : (q_{u_1}^{\text{nom}})^2 + 2q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} + 3q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} + (q_{u_2}^{\text{nom}})^2 + 3q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} \right. \\ &\quad \left. + 2(q_{u_3}^{\text{nom}})^2 \neq 0 \right\}. \end{aligned}$$

Direction 2: $Q_{0,a_1} = q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4} \geq 0$, $Q_{0,a_2} = q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4} - Q_{0,a_5} \geq 0$, $Q_{0,a_3} = q_{u_3}^{\text{nom}} - Q_{0,a_5} \leq 0$, $Q_{0,a_4} = z_1 \geq 0$, $Q_{0,a_5} = z_2 \geq 0$

Pressure drop polynomials:

$$\begin{aligned} h_1^{(2)} &= (q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1)^2 + (q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2)^2 - z_1^2 \\ h_2^{(2)} &= (q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2)^2 - (q_{u_3}^{\text{nom}} - z_2)^2 - z_2^2 \end{aligned}$$

Relevant branch of the comprehensive Gröbner system of $\langle h_1^{(2)}, h_2^{(2)} \rangle \subseteq \mathbb{R}[q_{u_1}^{\text{nom}}, q_{u_2}^{\text{nom}}, q_{u_3}^{\text{nom}}][z_1, z_2]$:

IF $q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} \neq 0$:

$$\begin{aligned} g_1^{(2)} &= 4z_2^4 + (8q_{u_1}^{\text{nom}} + 8q_{u_2}^{\text{nom}})z_2^3 + \left(-8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} - 16q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} - 8(q_{u_2}^{\text{nom}})^2 - 24q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} \right. \\ &\quad \left. - 8(q_{u_3}^{\text{nom}})^2 \right)z_2^2 + \left(4(q_{u_1}^{\text{nom}})^3 + 4(q_{u_1}^{\text{nom}})^2q_{u_2}^{\text{nom}} + 8(q_{u_1}^{\text{nom}})^2q_{u_3}^{\text{nom}} - 4q_{u_1}^{\text{nom}}(q_{u_2}^{\text{nom}})^2 \right. \\ &\quad \left. + 8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + 16q_{u_1}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 - 4(q_{u_2}^{\text{nom}})^3 + 16q_{u_2}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 + 8(q_{u_3}^{\text{nom}})^3 \right)z_2 \\ &\quad + (q_{u_1}^{\text{nom}})^4 - 2(q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}})^2 - 4(q_{u_1}^{\text{nom}})^2q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} - 4(q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}})^2 \\ &\quad - 8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 - 8q_{u_1}^{\text{nom}}(q_{u_3}^{\text{nom}})^3 + (q_{u_2}^{\text{nom}})^4 + 4(q_{u_2}^{\text{nom}})^3q_{u_3}^{\text{nom}} \\ &\quad - 8q_{u_2}^{\text{nom}}(q_{u_3}^{\text{nom}})^3 - 4(q_{u_3}^{\text{nom}})^4 \\ g_2^{(2)} &= (2q_{u_1}^{\text{nom}} + 2q_{u_2}^{\text{nom}} + 2q_{u_3}^{\text{nom}})z_1 - 2z_2^2 + 2q_{u_3}^{\text{nom}}z_2 - (q_{u_1}^{\text{nom}})^2 - 2q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} - 2q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} \\ &\quad - (q_{u_2}^{\text{nom}})^2 - 2q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} - 2(q_{u_3}^{\text{nom}})^2 \end{aligned}$$

The four roots of $g_1^{(2)} = 0$, $g_2^{(2)} = 0$ of this branch are $(Q_{0,a_4}^{(2,i)}(q^{\text{nom}}), Q_{0,a_5}^{(2,i)}(q^{\text{nom}}))$

for $i = 1, \dots, 4$ with

$$\begin{aligned}
Q_{0,a_5}^{(2,i)}(q^{\text{nom}}) &:= \text{Root}_i \text{ Of } \left(4z_2^4 + (8q_{u_1}^{\text{nom}} + 8q_{u_2}^{\text{nom}})z_2^3 + (-8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} - 16q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} \right. \\
&\quad \left. - 8(q_{u_2}^{\text{nom}})^2 - 24q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} - 8(q_{u_3}^{\text{nom}})^2 \right) z_2^2 + \left(4(q_{u_1}^{\text{nom}})^3 + 4(q_{u_1}^{\text{nom}})^2q_{u_2}^{\text{nom}} \right. \\
&\quad \left. + 8(q_{u_1}^{\text{nom}})^2q_{u_3}^{\text{nom}} - 4q_{u_1}^{\text{nom}}(q_{u_2}^{\text{nom}})^2 + 8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + 16q_{u_1}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 \right. \\
&\quad \left. - 4(q_{u_2}^{\text{nom}})^3 + 16q_{u_2}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 + 8(q_{u_3}^{\text{nom}})^3 \right) z_2 + (q_{u_1}^{\text{nom}})^4 - 2(q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}})^2 \\
&\quad - 4(q_{u_1}^{\text{nom}})^2q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} - 4(q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}})^2 - 8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 \\
&\quad \left. - 8q_{u_1}^{\text{nom}}(q_{u_3}^{\text{nom}})^3 + (q_{u_2}^{\text{nom}})^4 + 4(q_{u_2}^{\text{nom}})^3q_{u_3}^{\text{nom}} - 8q_{u_2}^{\text{nom}}(q_{u_3}^{\text{nom}})^3 - 4(q_{u_3}^{\text{nom}})^4 \right) \\
Q_{0,a_4}^{(2,i)}(q^{\text{nom}}) &:= \frac{1}{2(q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}})} \left(2(Q_{0,a_5}^{(2,i)}(q^{\text{nom}}))^2 - 2q_{u_3}^{\text{nom}}Q_{0,a_5}^{(2,i)}(q^{\text{nom}}) + (q_{u_1}^{\text{nom}})^2 \right. \\
&\quad \left. + 2q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} + 2q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} + (q_{u_2}^{\text{nom}})^2 + 2q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + 2(q_{u_3}^{\text{nom}})^2 \right)
\end{aligned}$$

The set of feasible load vectors that indicate a gas flow according to the second direction is

$$M^{(2)} := \bigcup_{i=1}^4 \left(X^{(2,i)} \cap Z^{(2,i)} \right) \cap Y^{(2)} \cap \{q^{\text{nom}+} : \mathbf{1}^T q^{\text{nom}+} = 0\}$$

with

$$\begin{aligned}
X^{(2,i)} &:= \left\{ q^{\text{nom}+} : q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4}^{(2,i)}(q^{\text{nom}}) \geq 0, q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4}^{(2,i)}(q^{\text{nom}}) \right. \\
&\quad \left. - Q_{0,a_5}^{(2,i)}(q^{\text{nom}}) \geq 0, q_{u_3}^{\text{nom}} - Q_{0,a_5}^{(2,i)}(q^{\text{nom}}) \leq 0, Q_{0,a_4}^{(2,i)}(q^{\text{nom}}) \geq 0, \right. \\
&\quad \left. Q_{0,a_5}^{(2,i)}(q^{\text{nom}}) \geq 0 \right\}, \\
Y^{(2)} &:= \{q^{\text{nom}+} : q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} \neq 0\}, \\
Z^{(2,i)} &:= Z(Q_{0,a_4}^{(2,i)}, Q_{0,a_5}^{(2,i)}).
\end{aligned}$$

Direction 3: $Q_{0,a_1} = q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4} \geq 0$, $Q_{0,a_2} = q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4} - Q_{0,a_5} \leq 0$, $Q_{0,a_3} = q_{u_3}^{\text{nom}} - Q_{0,a_5} \geq 0$, $Q_{0,a_4} = z_1 \geq 0$, $Q_{0,a_5} = z_2 \geq 0$

Pressure drop polynomials:

$$\begin{aligned}
h_1^{(3)} &= \left(q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 \right)^2 - \left(q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2 \right)^2 - z_1^2 \\
h_2^{(3)} &= - \left(q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2 \right)^2 + \left(q_{u_3}^{\text{nom}} - z_2 \right)^2 - z_2^2
\end{aligned}$$

Relevant branch of the comprehensive Gröbner system of $\langle h_1^{(3)}, h_2^{(3)} \rangle \subseteq$

$\mathbb{R}[q_{u_1}^{\text{nom}}, q_{u_2}^{\text{nom}}, q_{u_3}^{\text{nom}}][z_1, z_2]$:

$$\begin{aligned}
& \text{IF } (q_{u_1}^{\text{nom}})^2 + 2q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} + 3q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} + (q_{u_2}^{\text{nom}})^2 + 3q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + 2(q_{u_3}^{\text{nom}})^2 \neq 0: \\
g_1^{(3)} &= \left(4(q_{u_1}^{\text{nom}})^2 + 8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} + 16q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} + 4(q_{u_2}^{\text{nom}})^2 + 16q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + 16(q_{u_3}^{\text{nom}})^2\right) z_2^2 \\
&+ \left(4(q_{u_1}^{\text{nom}})^3 + 4(q_{u_1}^{\text{nom}})^2q_{u_2}^{\text{nom}} + 16(q_{u_1}^{\text{nom}})^2q_{u_3}^{\text{nom}} - 4q_{u_1}^{\text{nom}}(q_{u_2}^{\text{nom}})^2 + 8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}}\right. \\
&+ 8q_{u_1}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 - 4(q_{u_2}^{\text{nom}})^3 - 8(q_{u_2}^{\text{nom}})^2q_{u_3}^{\text{nom}} - 8q_{u_2}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 - 8(q_{u_3}^{\text{nom}})^3\left.) z_2\right. \\
&+ (q_{u_1}^{\text{nom}})^4 - 2(q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}})^2 - 4(q_{u_1}^{\text{nom}})^2q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} - 8(q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}})^2 \\
&- 8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 - 8q_{u_1}^{\text{nom}}(q_{u_3}^{\text{nom}})^3 + (q_{u_2}^{\text{nom}})^4 + 4(q_{u_2}^{\text{nom}})^3q_{u_3}^{\text{nom}} + 4(q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}})^2 \\
g_2^{(3)} &= (2q_{u_1}^{\text{nom}} + 2q_{u_2}^{\text{nom}} + 2q_{u_3}^{\text{nom}}) z_1 - 2q_{u_3}^{\text{nom}} z_2 - (q_{u_1}^{\text{nom}})^2 - 2q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} - 2q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} \\
&- (q_{u_2}^{\text{nom}})^2 - 2q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}}
\end{aligned}$$

The two roots of $g_1^{(3)} = 0$, $g_2^{(3)} = 0$ of this branch are $(Q_{0,a_4}^{(3,i)}(q^{\text{nom}}), Q_{0,a_5}^{(3,i)}(q^{\text{nom}}))$ for $i = 1, 2$ with

$$\begin{aligned}
Q_{0,a_5}^{(3,i)}(q^{\text{nom}}) &:= \frac{1}{2 \left((q_{u_1}^{\text{nom}})^2 + 2q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} + 4q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} + (q_{u_2}^{\text{nom}})^2 + 4q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + 4(q_{u_3}^{\text{nom}})^2 \right)} \\
&\left((-1)^i 2\sqrt{q_{u_3}^{\text{nom}}(q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}})^3} \right. \\
&\left. \sqrt{(q_{u_1}^{\text{nom}})^2 + 3q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} - (q_{u_2}^{\text{nom}})^2 - q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + (q_{u_3}^{\text{nom}})^2} \right. \\
&+ q_{u_1}^{\text{nom}}(q_{u_2}^{\text{nom}})^2 - (q_{u_1}^{\text{nom}})^2q_{u_2}^{\text{nom}} - 2q_{u_1}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 - 4(q_{u_1}^{\text{nom}})^2q_{u_3}^{\text{nom}} \\
&+ 2q_{u_2}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 + 2(q_{u_2}^{\text{nom}})^2q_{u_3}^{\text{nom}} - (q_{u_1}^{\text{nom}})^3 + (q_{u_2}^{\text{nom}})^3 + 2(q_{u_3}^{\text{nom}})^3 \\
&\left. - 2q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} \right) \\
Q_{0,a_4}^{(3,i)}(q^{\text{nom}}) &:= \frac{1}{2(q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}})} \left(2q_{u_3}^{\text{nom}}Q_{0,a_5}^{(3,i)}(q^{\text{nom}}) + (q_{u_1}^{\text{nom}})^2 + 2q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} \right. \\
&\left. + 2q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} + (q_{u_2}^{\text{nom}})^2 + 2q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} \right)
\end{aligned}$$

The set of feasible load vectors that indicate a gas flow according to the third direction is

$$M^{(3)} := \bigcup_{i=1,2} \left(X^{(3,i)} \cap Z^{(3,i)} \right) \cap Y^{(3)} \cap \{q^{\text{nom}+} : \mathbf{1}^T q^{\text{nom}+} = 0\}$$

with

$$\begin{aligned}
X^{(3,i)} &:= \left\{ q^{\text{nom}+} : q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4}^{(3,i)}(q^{\text{nom}}) \geq 0, q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4}^{(3,i)}(q^{\text{nom}}) \right. \\
&- Q_{0,a_5}^{(3,i)}(q^{\text{nom}}) \leq 0, q_{u_3}^{\text{nom}} - Q_{0,a_5}^{(3,i)}(q^{\text{nom}}) \geq 0, Q_{0,a_4}^{(3,i)}(q^{\text{nom}}) \geq 0, \\
&\left. Q_{0,a_5}^{(3,i)}(q^{\text{nom}}) \geq 0 \right\}, \\
Y^{(3)} &:= \left\{ q^{\text{nom}+} : (q_{u_1}^{\text{nom}})^2 + 2q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} + 3q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} + (q_{u_2}^{\text{nom}})^2 + 3q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} \right. \\
&\left. + 2(q_{u_3}^{\text{nom}})^2 \neq 0 \right\}, \\
Z^{(3,i)} &:= Z \left(Q_{0,a_4}^{(3,i)}, Q_{0,a_5}^{(3,i)} \right).
\end{aligned}$$

Direction 4: $Q_{0,a_1} = q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4} \geq 0$, $Q_{0,a_2} = q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4} - Q_{0,a_5} \leq 0$, $Q_{0,a_3} = q_{u_3}^{\text{nom}} - Q_{0,a_5} \geq 0$, $Q_{0,a_4} = z_1 \geq 0$, $Q_{0,a_5} = z_2 \leq 0$

Pressure drop polynomials:

$$h_1^{(4)} = \left(q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 \right)^2 - \left(q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2 \right)^2 - z_1^2$$

$$h_2^{(4)} = - \left(q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - z_1 - z_2 \right)^2 + \left(q_{u_3}^{\text{nom}} - z_2 \right)^2 + z_2^2$$

Relevant branch of the comprehensive Gröbner system of $\langle h_1^{(4)}, h_2^{(4)} \rangle \subseteq \mathbb{R}[q_{u_1}^{\text{nom}}, q_{u_2}^{\text{nom}}, q_{u_3}^{\text{nom}}][z_1, z_2]$:

IF $q_1 + q_2 + q_3 \neq 0$:

$$g_1^{(4)} = 4z_2^4 + (-8q_{u_1}^{\text{nom}} - 8q_{u_2}^{\text{nom}} - 16q_{u_3}^{\text{nom}})z_2^3 + \left(-8(q_{u_1}^{\text{nom}})^2 - 8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} + 8q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + 16(q_{u_3}^{\text{nom}})^2 \right)z_2^2 + \left(4(q_{u_1}^{\text{nom}})^3 + 4(q_{u_1}^{\text{nom}})^2q_{u_2}^{\text{nom}} + 16(q_{u_1}^{\text{nom}})^2q_{u_3}^{\text{nom}} - 4q_{u_1}^{\text{nom}}(q_{u_2}^{\text{nom}})^2 + 8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + 8q_{u_1}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 - 4(q_{u_2}^{\text{nom}})^3 - 8(q_{u_2}^{\text{nom}})^2q_{u_3}^{\text{nom}} - 8q_{u_2}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 - 8(q_{u_3}^{\text{nom}})^3 \right)z_2 + (q_{u_1}^{\text{nom}})^4 - 2(q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}})^2 - 4(q_{u_1}^{\text{nom}})^2q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} - 8(q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}})^2 - 8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 - 8q_{u_1}^{\text{nom}}(q_{u_3}^{\text{nom}})^3 + (q_{u_2}^{\text{nom}})^4 + 4(q_{u_2}^{\text{nom}})^3q_{u_3}^{\text{nom}} + 4(q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}})^2$$

$$g_2^{(4)} = (2q_{u_1}^{\text{nom}} + 2q_{u_2}^{\text{nom}} + 2q_{u_3}^{\text{nom}})z_1 + 2z_2^2 - 2q_{u_3}^{\text{nom}}z_2 - (q_{u_1}^{\text{nom}})^2 - 2q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} - 2q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} - (q_{u_2}^{\text{nom}})^2 - 2q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}}$$

The four roots of $g_1^{(4)} = 0$, $g_2^{(4)} = 0$ of this branch are $(Q_{0,a_4}^{(4,i)}(q^{\text{nom}}), Q_{0,a_5}^{(4,i)}(q^{\text{nom}}))$ for $i = 1, \dots, 4$ with

$$Q_{0,a_5}^{(4,i)}(q^{\text{nom}}) := \text{Root}_i \text{ Of } \left(4z_2^4 + (-8q_{u_1}^{\text{nom}} - 8q_{u_2}^{\text{nom}} - 16q_{u_3}^{\text{nom}})z_2^3 + \left(-8(q_{u_1}^{\text{nom}})^2 - 8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} + 8q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + 16(q_{u_3}^{\text{nom}})^2 \right)z_2^2 + \left(4(q_{u_1}^{\text{nom}})^3 + 4(q_{u_1}^{\text{nom}})^2q_{u_2}^{\text{nom}} + 16(q_{u_1}^{\text{nom}})^2q_{u_3}^{\text{nom}} - 4q_{u_1}^{\text{nom}}(q_{u_2}^{\text{nom}})^2 + 8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} + 8q_{u_1}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 - 4(q_{u_2}^{\text{nom}})^3 - 8(q_{u_2}^{\text{nom}})^2q_{u_3}^{\text{nom}} - 8q_{u_2}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 - 8(q_{u_3}^{\text{nom}})^3 \right)z_2 + (q_{u_1}^{\text{nom}})^4 - 2(q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}})^2 - 4(q_{u_1}^{\text{nom}})^2q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} - 8(q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}})^2 - 8q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}}(q_{u_3}^{\text{nom}})^2 - 8q_{u_1}^{\text{nom}}(q_{u_3}^{\text{nom}})^3 + (q_{u_2}^{\text{nom}})^4 + 4(q_{u_2}^{\text{nom}})^3q_{u_3}^{\text{nom}} + 4(q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}})^2 \right)$$

$$Q_{0,a_4}^{(4,i)}(q^{\text{nom}}) := \frac{1}{2(q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}})} \left(-2Q_{0,a_5}^{(4,i)}(q^{\text{nom}})^2 + 2q_3^{\text{nom}}Q_{0,a_5}^{(4,i)}(q^{\text{nom}}) + (q_{u_1}^{\text{nom}})^2 + 2q_{u_1}^{\text{nom}}q_{u_2}^{\text{nom}} + 2q_{u_1}^{\text{nom}}q_{u_3}^{\text{nom}} + (q_{u_2}^{\text{nom}})^2 + 2q_{u_2}^{\text{nom}}q_{u_3}^{\text{nom}} \right)$$

The set of feasible load vectors that indicate a gas flow according to the fourth direction is

$$M^{(4)} := \bigcup_{i=1}^4 \left(X^{(4,i)} \cap Z^{(4,i)} \right) \cap Y^{(4)} \cap \left\{ q^{\text{nom}+} : \mathbf{1}^T q^{\text{nom}+} = 0 \right\}$$

with

$$\begin{aligned}
X^{(4,i)} &:= \left\{ q^{\text{nom}+} : q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4}^{(4,i)}(q^{\text{nom}}) \geq 0, q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} - Q_{0,a_4}^{(4,i)}(q^{\text{nom}}) \right. \\
&\quad \left. - Q_{0,a_5}^{(4,i)}(q^{\text{nom}}) \leq 0, q_{u_3}^{\text{nom}} - Q_{0,a_5}^{(4,i)}(q^{\text{nom}}) \geq 0, Q_{0,a_4}^{(4,i)}(q^{\text{nom}}) \geq 0, \right. \\
&\quad \left. Q_{0,a_5}^{(4,i)}(q^{\text{nom}}) \leq 0 \right\}, \\
Y^{(4)} &:= \left\{ q^{\text{nom}+} : q_{u_1}^{\text{nom}} + q_{u_2}^{\text{nom}} + q_{u_3}^{\text{nom}} \neq 0 \right\}, \\
Z^{(4,i)} &:= Z \left(Q_{0,a_4}^{(4,i)}, Q_{0,a_5}^{(4,i)} \right).
\end{aligned}$$

As a conclusion, M can be restated as

$$M = \bigcup_{j=1}^4 M^{(j)}.$$

Part III
Appendix

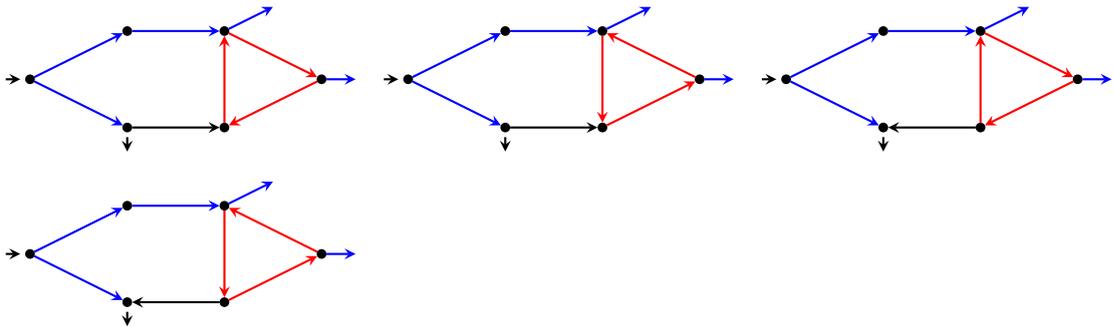
Appendix A

Extension of Examples Concerning Flow Directions

A.1 Infeasible Flow Directions of Example 5.9

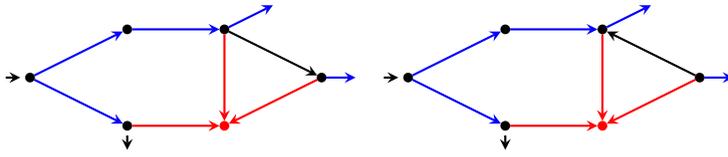
Figure A.1 contains infeasible flow directions of the subgraph in Example 5.9. The flow direction along arcs that are depicted in blue are already fixed. The flows along the remaining arcs can be directed in $2^4 = 16$ different ways, but only the infeasible ones are shown in Figure A.1. The arcs which lead to infeasibility of the flow direction are depicted in red.

In Figure A.1(a) the red arcs compose a cycle that is directed w.r.t. the flow direction which contradicts (iv) of Proposition 5.7. The out-degree of the red node in Figure A.1(b) and the in-degree of the red node in Figure A.1(c) and Figure A.1(d) is zero, in contradiction to (iii) of Proposition 5.7.

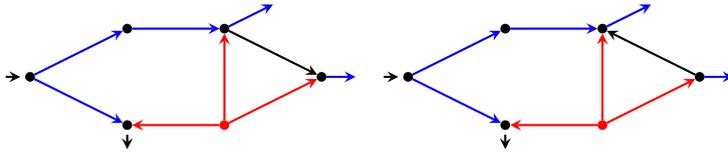


(a) Directed Cycles

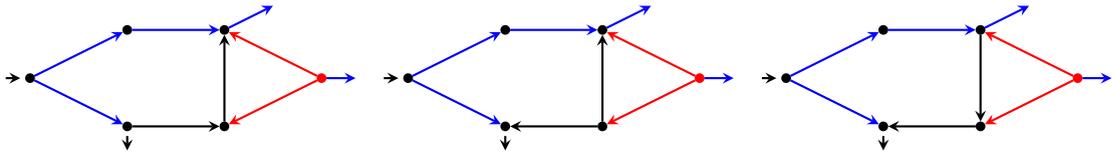
Figure A.1: Infeasible Flow Directions of Example 5.9.



(b) Out-degree at the Red Node is Zero



(c) In-degree at the Red Node is Zero



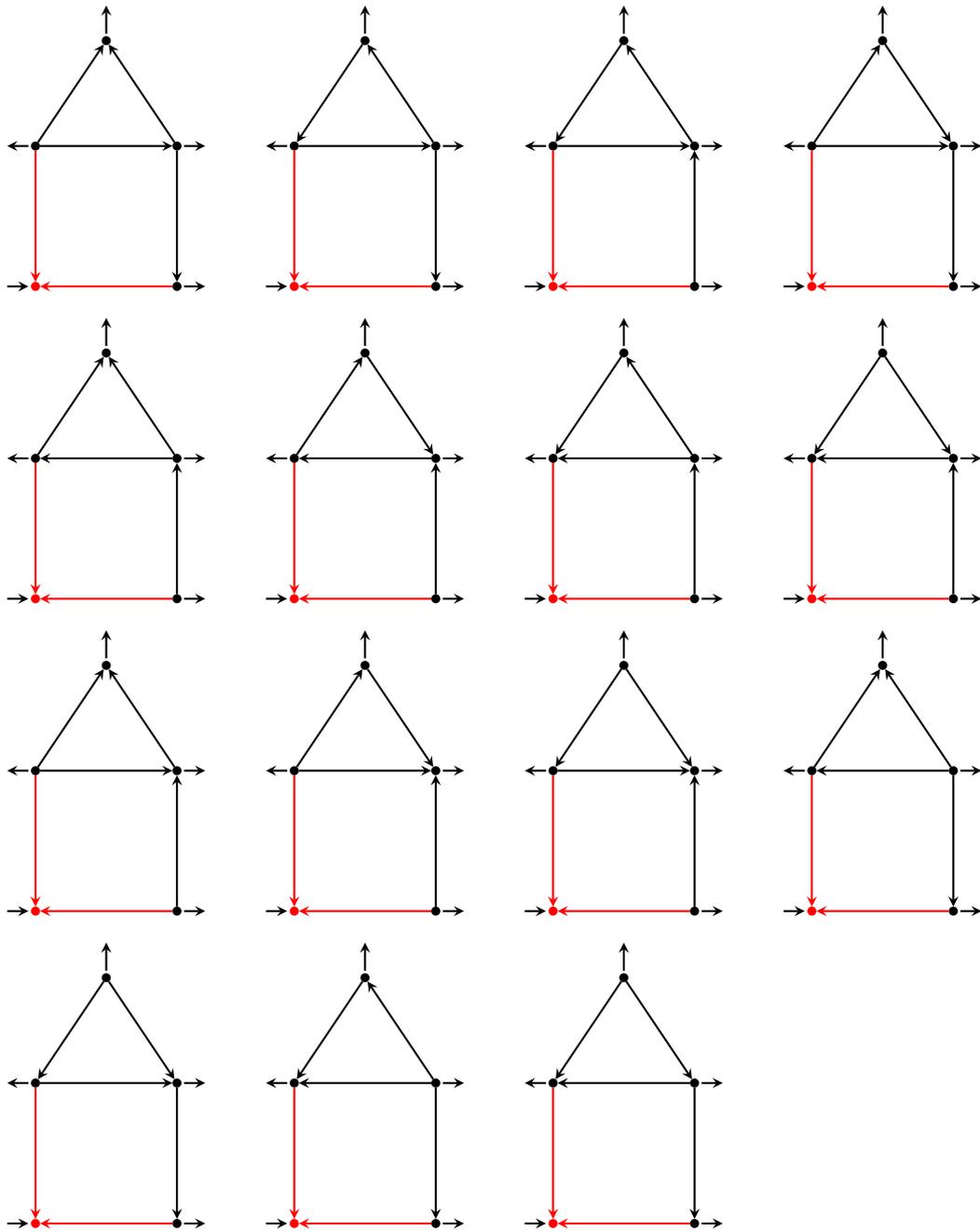
(d) In-degree at the Red Node is Zero

Figure A.1: Infeasible Flow Directions of Example 5.9. (cont.)

A.2 Infeasible Flow Directions of Example 5.15

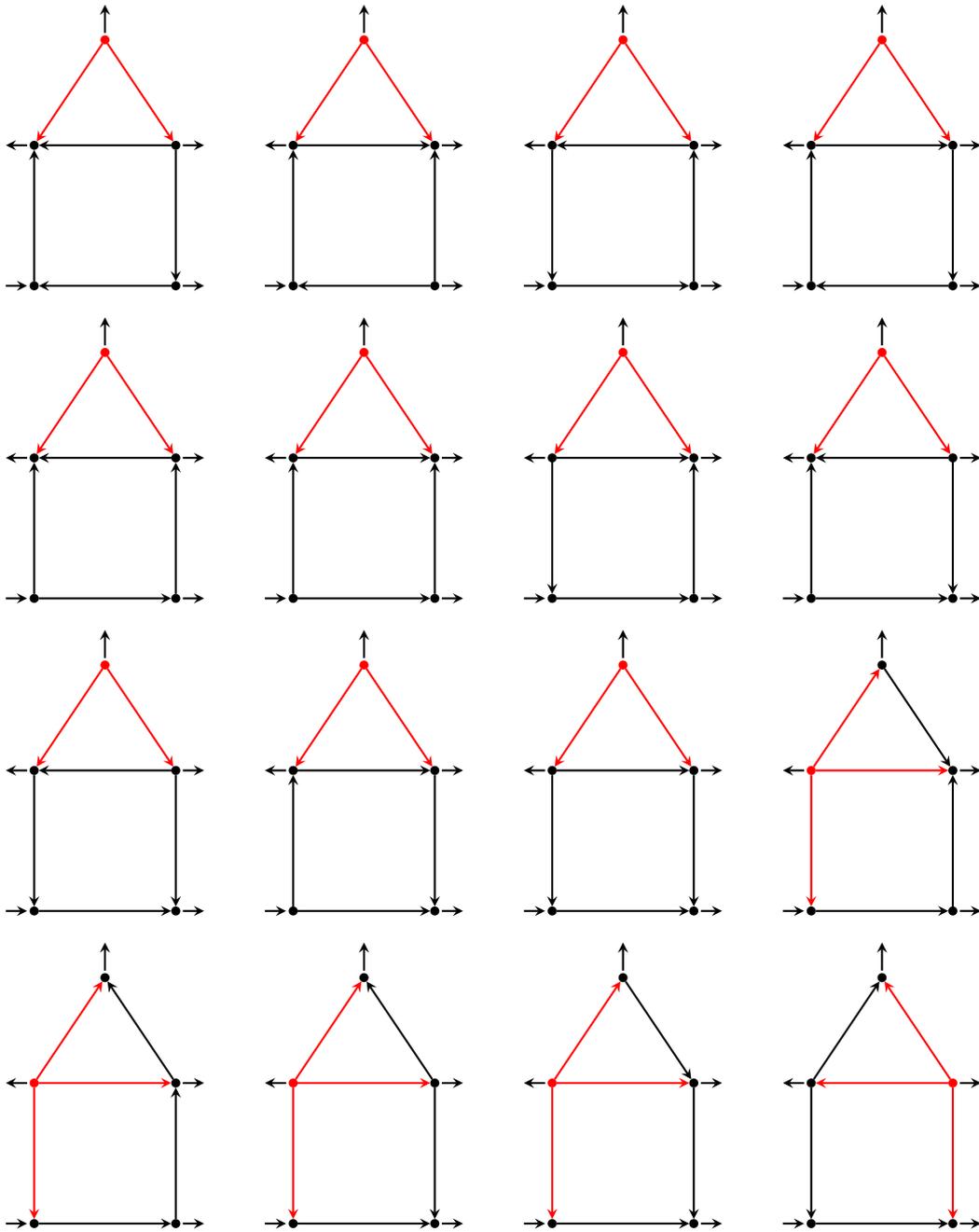
Figure A.2 contains infeasible flow directions of the network in Example 5.15. The flows along the arcs can be directed in $2^6 = 64$ different ways, but only the ones violating (i) or (ii) of Proposition 5.7 or failing to serve every exit node are shown in Figure A.2. The arcs which lead to infeasibility of the flow direction are depicted in red.

The out-degree of the red node in Figure A.2(a) and the in-degree of the red node in Figure A.2(b) is zero, in contradiction to (i) and (ii) of Proposition 5.7, respectively. In Figure A.2(c) the red nodes are not reached by the gas.



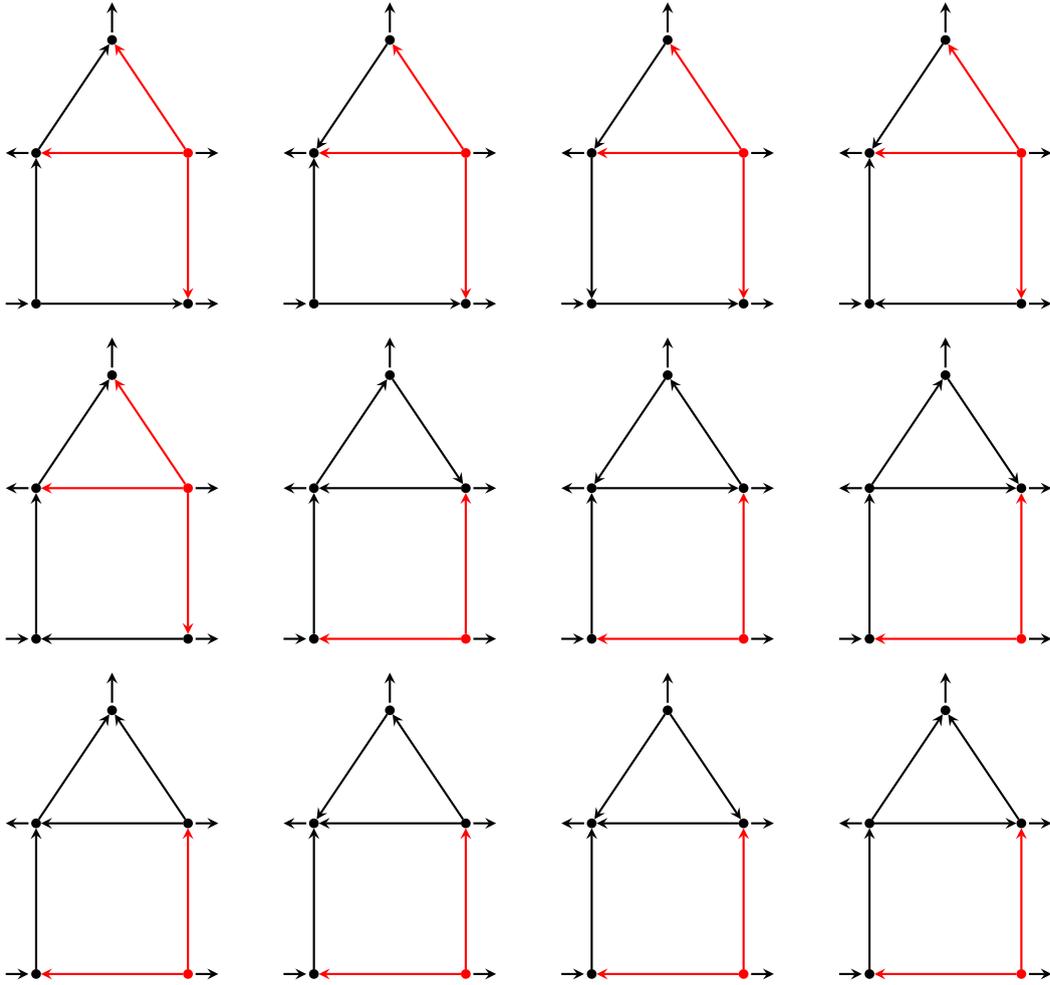
(a) Out-degree at the Red Entry Node is Zero

Figure A.2: Infeasible Flow Directions of Example 5.15.

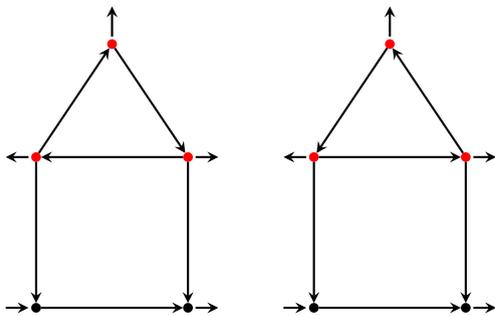


(b) In-degree at the Red Exit Node is Zero

Figure A.2: Infeasible Flow Directions of Example 5.15. (cont.)



(b) In-degree at the Red Exit Node is Zero (cont.)



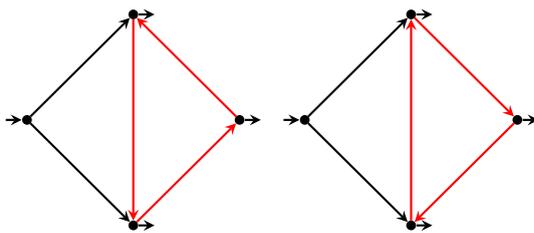
(c) Red Nodes are Not Reached

Figure A.2: Infeasible Flow Directions of Example 5.15. (cont.)

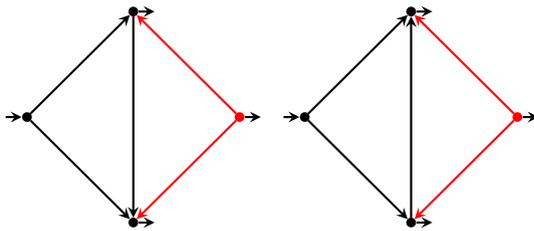
A.3 Infeasible Flow Directions of Example 7.2

Figure A.3 contains infeasible flow directions of the network in Example 7.2. After fixing the flow along the arcs incident to the unique entry node u_0 the flows along the remaining arcs can be directed in $2^3 = 8$ different ways, but only the ones violating the rules of Proposition 5.7 are shown in Figure A.3. The arcs which lead to infeasibility of the flow direction are depicted in red.

In Figure A.3(a) the red arcs compose a cycle that is directed w.r.t. the flow direction which contradicts (iv) of Proposition 5.7. The in-degree of the red node in Figure A.3(b) is zero, in contradiction to (ii) of Proposition 5.7.



(a) Directed Cycle



(b) In-degree at the Red Exit Node is Zero

Figure A.3: Infeasible Flow Directions of Example 7.2.

Appendix B

Data

Tables B.1 – B.3 contain the data of the networks used for the computations in Section 6.2.

	2 Cycles	3 Cycles
Entry	[50, 60]	[50, 60]
Exit ₁	[57, 60]	[57, 60]
Exit ₂	[57, 60]	[58, 60]
Innode ₁	[2, 100]	[2, 100]
Innode ₂	–	[2, 100]

Table B.1: Pressure Bounds at the Nodes in Bar.

	2 Cycles	3 Cycles
a_1	0.00039685	0.00039685
a_2	0.00039648	0.00039648
a_3	0.00039666	0.00039515
a_4	0.00039631	0.00039617
a_5	0.00039614	0.00039581
a_6	–	0.00040323
a_7	–	0.00039614

Table B.2: Pressure Drop Coefficients of the Arcs.

	2 Cycles	3 Cycles
Exit ₁	14	10
Exit ₂	16	60

Table B.3: Mean value of the Distribution of the Loads at the Exits in $1000 \text{ m}^3 \text{ h}^{-1}$.

	2 Cycles	3 Cycles
Exit ₁	1	100
Exit ₂	100	100

Table B.4: Variance of the Exit Loads.

For this tests it is assumed that the exit loads at the distinct exit nodes are uncorrelated. Hence, the covariance matrix is a diagonal matrix whose nonzero entries are the variances of the exit loads. The variances are listed in Table B.4.

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