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Topological solvability and DAE-index conditions for types of black-box models coupled to liquid flow networks via boundary conditions

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Abstract This work is devoted to the analysis of fluid networks stemming from automated modeling processes in system simulation software. Today's system modeling software typically offers a wide range of basic physical components (e.g. pumps, pipes), which can be assembled to customized physical networks simply by drag and drop. The governing equations are derived by representing the network as a linear graph whose edges and nodes correspond to the basic physical components. Combining the connection structure of the graph with the physical equations of the components, the physical network is modeled as Differential-Algebraic Equations (DAE). Using algebraic graph and DAE theory, the solvability of the mathematical model can be analyzed and translated as conditions on the network structure and properties of its elements. To control these networks or to connect them to the environment, boundary conditions are present, allowing to incorporate user defined components. In many practical applications, these external components (e.g. controllers) are given by black-box models. Recently the Functional Mock-up Unit (FMU) has been established as a standardized structured interface for those kinds of black-box models, giving the input-output relation as differential state and algebraic output equation. Incorporating these types of black-box components into physical networks may drastically affect its physical validity and solvability. Within this work, a coupled DAE-FMU system is analyzed and conditions on the network structure, its elements and the coupled FMUs are presented, that allow to preserve the physical validity as well as the solvability of the physical network. Keeping a close connection between the topology of the model and the equations of the network, the solvability conditions of the model can be interpreted as easy-to-check graph theoretical conditions on the network and the FMUs, which can significantly increase the usability of such system simulation processes for fluid networks.

Keywords differential-algebraic equation · topological index criteria · hydraulic network · coupled system · modified nodal analysis · functional mock-up interface

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1 Introduction

Increasingly demanding emissions legislation specifies the performance requirements for the next generation of products from vehicle manufacturers. Conversely, the increasingly stringent emissions legislation is coupled with the trend in increased power, drivability and safety expectations from the consumer market. Promising approaches to meet these requirements are downsizing the internal combustion engines (ICE), the application of turbochargers, variable valve timing, advanced combustion systems or comprehensive exhaust aftertreatment but also different variants of combinations of the ICE with an electrical engine in terms of hybridization or even a purely electric propulsion. The challenges in the development of future powertrains do not only lie in the design of individual components but in the assessment of the powertrain as a whole. On a system engineering level it is required to optimize individual components globally and to balance the interaction of different subsystems. A typical system engineering model comprises several sub-systems. For instance, in case of a hybrid propulsion these can be the vehicle chassis, the drive line, the air path of the ICE including combustion and exhaust aftertreatment, the cooling and lubrication system of the ICE and battery packs, the electrical propulsion system including the engine and a battery pack, the air conditioning and passenger cabin models, waste heat recovery and finally according control systems.

State-of-the-art modeling and simulation packages such as Dymola[1], OpenModelica[2], Matlab/Simulink[3], Flowmaster[4], Amesim[5], SimulationX[6], or Cruise M[7] offer many concepts for the automatic generation of dynamic system models. Modeling is done in a modularized way, based on a network of subsystems which again consists of simple standardized subcomponents. The automated modeling process allows the usage of various advanced libraries for different subcomponents of the system from possibly different physical domains. The connections between those subcomponents are typically based on physical coupling conditions or predefined controller interfaces. Furthermore the network structure (topology) carries the core information of the network properties and therefore is predestinated to be exploited for the analysis and numerical simulation of those. In the application of vehicle system simulation the equations of the subsystems are differential-algebraic equations (DAE) of higher index. Hence, this type of modeling leads to systems of coupled large DAE-systems. Consequently, the analysis of existence and uniqueness of solutions for both, the individual physical subsystems and the full coupled system of DAE-systems, is a delicate issue.

Topology based index analysis for networks connects the research fields of *Analysis for DAEs* [18] and *Graph Theory* [6] in order to provide the appropriate base to analyze DAEs stemming from automatic generated system models. So far it has been established for various types of networks, including electric circuits [21] (*Modified Nodal Analysis*), gas supply networks [7], thermal liquid flow networks [1,2] and water supply networks [8,9,19]. Although all those networks share some similarities, an individual investigation is required due to their different physical nature. Recently, a unified modeling approach for different types of flow networks has been introduced in [10], aiming for a unified topology based index analysis for the different physical domains on an abstract level. In the mentioned approaches, the analysis of the different physical domains is always restricted to a simple connected network of one physical type. Anyhow, all the approaches have in common, that they provide an index reduced (differential-index (d-index) 1 or strangeness-index (s-index) 0, cf. [16]) formulation of the original DAE, which is suitable for numerical integration.

Due to the increasing complexity in vehicle system simulation the interchangeability of submodels is gaining increasing importance. Submodels are exchanged between different simulation environ-

[1] http://www.dynasim.com
[2] http://www.openmodelica.org
[3] http://www.mathworks.com
[4] http://www.mentor.com
[5] http://www.plm.automation.siemens.com
[6] http://www.iti.de
[7] http://www.avl.com

ments in terms of white-box or black-box libraries describing a set of DAEs. The interconnection to the system of physical based DAEs is again established by predefined controller interface or physical coupling conditions. The individual subnetworks are assumed to be of index reduced form (d-index 1 or s-index 0). This can be achieved by the *Topological index analysis* or *Modified Nodal Analysis*. It is well known [17], that the combination of d-index 1 DAEs may not form a d-index 1 DAE.

A first attempt to couple various circuits of the same physical type (liquid flow) via coupling conditions is presented in [3]. At the first glance, the artificial coupling of circles of the same physical type via (defined) physical coupling conditions within one simulation package might appear superfluous, since the circuit could be modeled all at once. But due to increasing complexity also within one physical domain, the modeling of subcircuits is distributed among high specialized teams and finally combined to the complete circuit. Using physical coupling conditions allows to combine the subcircuits to a single circuit without modifying the developed submodels. For the case of DAEs of higher index, this is of special importance, since the set of feasible initial conditions is often defined by structural properties (e.g. chord sets or spanning trees) and they might change in a coupling process. Due to integrity of the overall modeling process, this type of change should be avoided. Typically, the physical coupling conditions are defined to ensure that certain conservation laws are satisfied, e.g. conservation of mass in liquid flow networks or conservation of charge in electric systems. Consequently, an appropriate treatment of those coupling conditions is a delicate issue.

A natural extension of this scenario is the following. If the protection of intellectual property of a specific subcircuit model is of high priority, the specific part can be incorporated in a black-box model. Although the actual physical content is not known, educated guesses based on the offered connection points allow to apply physical based rules to the coupling interface. Therein it is assumed that the black box model fulfills certain requirements and offers a suitable pair of ports, which allows to build up a feasible connection to the coupling interface. Examples for black box model with user defined content, but framework defined physical connections can be found, e.g., in Cruise M[8].

One very recent example in automotive applications is the incorporation of black-boxes in the form of so-called *Functional Mock-Up Units* (FMUs) in physical networks. The *Functional Mock-up Interface* (FMI)[9] provides a tool independent standard to support model exchange of subsystems. On the one hand those black-box approaches promote the possibility for hiding intellectual property and guarantee platform independence, but on the other hand they raise the challenge to incorporate those systems in the automated modeling and simulation process of multi-physics dynamical systems.

The incorporation of FMUs is of special interest in the context of *Topology based index analysis* or *Modified Nodal Analysis*, since it allows to extract additional information due to the knowledge of the underlying physics. Furthermore, the FMUs provide additional information in form of internal dependency graphs of their inputs and outputs. Indeed at that point it is required to link purely graph theoretical approaches with physical based topological methods in order to extract the advantages of both worlds.

In the following we address the case of liquid flow networks coupled with various FMUs via defined boundary conditions and explore the physical properties (e.g. conservation laws) of the system to derive topological based index and solvability conditions. In [8] a unified modeling approach for different types of flow networks (electric circuits, water and gas networks) has been stated. One specific part of this classifications are the boundary conditions, that prescribe a certain pressure or potential for node elements and flow sources. In the case of electric networks, those elements are voltage sources and current sources. In the case of gas and liquid flow networks, those are reservoirs and demand branches. Those boundary conditions provide the starting point for defining appropriate coupling and interface conditions. As an example we explore the coupling for the case of a liquid flow network coupled to FMUs via reservoirs and demand branches. Providing pressure controlled flow sources and flow controlled pressure sources establishes a strong coupling of the individual liquid flow networks.

The structure of this work is the following. In Section 2 we state a simple model for an incompressible liquid flow network as developed in [2]. The concept of FMUs and their mathematical

[8] http://www.avl.com

[9] http://fmi-standard.org/

representation is introduced in Section 3. In Section 4 we state a coupled model of incompressible flow networks and FMUs and define appropriate coupling conditions. Section 5 is devoted to the definition of the graph theoretical prerequisites. Specific constellations in the liquid flow network are identified and the corresponding equation parts are analyzed. The results obtained in Section 5 are applied to the stated surrogate network function in Section 6 to obtain the final existence and uniqueness results, as well as strangeness index considerations of the resulting DAE in Section 7. Furthermore, a descriptive example describes the relevant results of this work. Finally, Section 9 provides an overview of the addressed issues. Therein another major focus is put on the description of open topics and further research requirements.

2 A network model for incompressible flow networks

We consider a liquid flow network

$$\mathcal{N} = \{\mathcal{PI}, \mathcal{PU}, \mathcal{DE}, \mathcal{JC}, \mathcal{RE}\}, \tag{1}$$

that is composed of pipes $\mathcal{PI} = \{\mathrm{Pi}_1, ..., \mathrm{Pi}_{n_{\mathrm{Pi}}}\}$, pumps $\mathcal{PU} = \{\mathrm{Pu}_1, ..., \mathrm{Pu}_{n_{\mathrm{Pu}}}\}$, demands $\mathcal{DE} = \{\mathrm{De}_1, ..., \mathrm{De}_{n_{\mathrm{De}}}\}$, junctions $\mathcal{JC} = \{\mathrm{Jc}_1, ..., \mathrm{Jc}_{n_{\mathrm{Jc}}}\}$ and reservoirs $\mathcal{RE} = \{\mathrm{Re}_1, ..., \mathrm{Re}_{n_{\mathrm{Re}}}\}$ and that is filled with an incompressible fluid. The pipes and pumps are connected by the junctions, where the fluid is split or merged. The connection to the environment is modeled by the reservoirs and demands that impose a predefined pressure or mass flow to the network.

To set up a mathematical model describing the mass flows in the pipes and pumps and the pressures in the junctions, the network $\mathcal{N}$ is represented by a linear graph $\mathcal{G}$. A linear graph $\mathcal{G}$ is a combination $\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$ of vertices $\mathcal{V} = \{v_1, ..., v_{n_\mathcal{V}}\}$ and edges $\mathcal{E} = \{e_1, ..., e_{n_\mathcal{E}}\}$, such that each edge $e_i \in \mathcal{E}$ corresponds to a pair of vertices $(v_{i_1}, v_{i_2}) \in \mathcal{V} \times \mathcal{V}$, i.e., $e_i = (v_{i_1}, v_{i_2})$, cp. [6, p. 2]. For a detailed introduction to graph theory, we refer the reader to, e.g., [4,6,20].

For the network $\mathcal{N}$, the pipes, pumps and demands correspond to the edges, i.e., $\mathcal{E} = \{\mathcal{PI}, \mathcal{PU}, \mathcal{DE}\}$, while the junctions and reservoirs correspond to the vertices, i.e., $\mathcal{V} = \{\mathcal{JC}, \mathcal{RE}\}$, cf. Figure 1. To each edge a mass flow and to each junction a pressure is assigned, denoted by q_{Pi_i}, q_{Pu_i}, q_{De_i} and p_{Jc_i} and p_{Re_i} depending on the type and number of the element. To specify the direction of the mass flows, the edges are directed, meaning that the pair $e_i = (v_{i_1}, v_{i_2}) \in \mathcal{E}$ is ordered. Then, the graph $\mathcal{G}$ is oriented.

We consider networks satisfying the following assumptions on their connection structure.

Assumption 1 *Consider a network $\mathcal{N}$ as in* (1).

(1) Two junctions are connected at most by one pipe or one pump.
(2) Each pipe, pump and demand has an assigned direction.
(3) The network is connected, i.e., every pair of junctions and/or reservoirs can be reached by a sequence of pipes and pumps.
(4) Every junction is adjacent to at most one demand branch. Every reservoir is connected at most to one pipe or pump.

Under Assumption 1 the network graph is simple (1), oriented (2) and connected (3). Reservoirs and demands are separated by at least two network elements (4).

The connection structure of the network $\mathcal{N}$ is described by the incidence matrix $A = (a_{ij})$, which is defined as, cp. e.g. [4,6,20],

$$a_{ij} = \begin{cases} 1, & \text{if the branch } j \text{ leaves the node } i, \\ -1, & \text{if the branch } j \text{ enters the node } i, \\ 0, & \text{else.} \end{cases}$$

Sorting the rows and columns of A according to the different element types, we obtain the incidence matrix as

$$A = \begin{bmatrix} A_{\mathrm{Jc,Pi}} & A_{\mathrm{Jc,Pu}} & A_{\mathrm{Jc,De}} \\ A_{\mathrm{Re,Pi}} & A_{\mathrm{Re,Pu}} & A_{\mathrm{Re,De}} \end{bmatrix}.$$

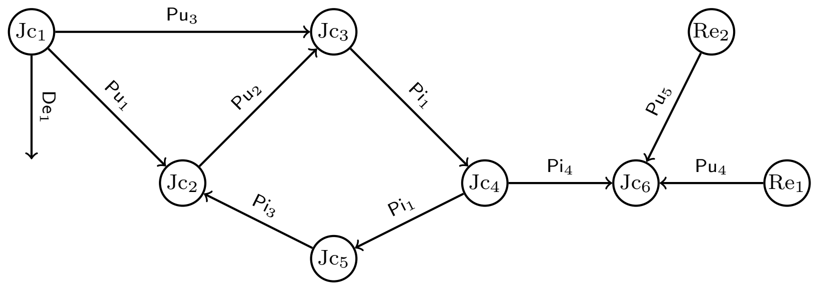


Fig. 1: Example of a graph $\mathcal{G}$ of a network $\mathcal{N}$.

Note that under Assumption 1, $A_{\mathrm{Re,De}} = 0$ and there exist permutations P_1, P_2 such that

$$[A_{\mathrm{Re,Pi}}, A_{\mathrm{Re,Pu}}]P_1 = [I_{\mathrm{Re}}, 0],$$
$$P_2^T A_{\mathrm{Jc,De}} = [I_{\mathrm{De}}, 0]^T.$$

The flows and pressures are summarized as

$$q = \begin{bmatrix} q_{\mathrm{Pi}} \\ q_{\mathrm{Pu}} \\ q_{\mathrm{De}} \end{bmatrix}, \quad p = \begin{bmatrix} p_{\mathrm{Jc}} \\ p_{\mathrm{Re}} \end{bmatrix}.$$

Besides the connection structure, each network element is equipped with a characteristic equation describing the relation of the mass flow and pressure or pressure difference. In a pipe Pi_i, $i = 1, ..., n_{\mathrm{Pi}}$, directed from node i_1 to node i_2, the mass flow q_{Pi_i} is specified by the transient momentum equation

$$\dot{q}_{\mathrm{Pi}_i} = c_{1,i} \Delta p_j + c_{2,i} |q_{\mathrm{Pi}_i}| q_{\mathrm{Pi}_i} + c_{3,i},$$

depending on the pressure difference $\Delta p_i = p_{i_1} - p_{i_2}$ between the adjacent nodes i_1, i_2 and constants $c_{k,i}$, $k = 1, 2, 3$, depending, e.g., on the pipe diameter, length, inclination angle, and other physical properties, cp. [3, Remark 1]. Using the incidence matrix A, the pressure drop $\Delta p_i = p_{i_1} - p_{i_2}$ along an edge $e_i = (v_{i_1}, v_{i_2})$ is given by $e_i^T A^T p = \Delta p_i$. Setting $C_k = \operatorname{diag}\left(c_{k,i}\right)_i$, $i = 1, ...n_{\mathrm{Pi}}$, $k = 1, 2, 3$, we define the *pipe function* $f_{\mathrm{Pi}} \colon \mathbb{R}^{n_{\mathrm{Pi}}} \times \mathbb{R}^{n_{\mathrm{Jc}}} \times \mathbb{R}^{n_{\mathrm{Re}}} \to \mathbb{R}^{n_{\mathrm{Pi}}}$ of the full network by

$$f_{\mathrm{Pi}}(q_{\mathrm{Pi}}, p_{\mathrm{Jc}}, p_{\mathrm{Re}}) := C_1(A_{\mathrm{Jc,Pi}}^T p_{\mathrm{Jc}} + A_{\mathrm{Re,Pi}}^T p_{\mathrm{Re}}) + C_2 \operatorname{diag}\left(|q_{\mathrm{Pi}_i}|\right)_j q_{\mathrm{Pi}} + C_3.$$

Then, the transient momentum equations for the whole network read

$$\dot{q}_{\mathrm{Pi}} = f_{\mathrm{Pi}}(q_{\mathrm{Pi}}, p_{\mathrm{Jc}}, p_{\mathrm{Re}}). \tag{2a}$$

In a pump Pu_i, $i = 1, ..., n_{\mathrm{Pu}}$, directed from node i_1 to node i_2, the mass flow q_{Pu_i} is specified algebraically by the pressure drop $\Delta p_i = p_{i_1} - p_{i_2}$, i.e.,

$$\Delta p_i = f_{\mathrm{Pu}_i}(q_{\mathrm{Pu}_i}).$$

The function f_{Pu_i} is given by specialized pump models, cp. [3, Remark 2]. Like for the pipes, we use the incidence matrix A to summarize the pump functions for the full network in the *pump function* $f_{\mathrm{Pu}} \colon \Omega_{\mathrm{Pu}} \to \mathbb{R}^{n_{\mathrm{Pu}}}$ given by

$$f_{\mathrm{Pu}} := [f_{\mathrm{Pu}_i}]_{i=1,...,n_{\mathrm{Pu}}},$$

where $\Omega_{\mathrm{Pu}} \subset \mathbb{R}^{n_{\mathrm{Pu}}}$ denotes the set of admissible pump flows. Then, the pump equations for the whole network read

$$A_{\mathrm{Jc,Pu}}^T p_{\mathrm{Jc}} + A_{\mathrm{Re,Pu}}^T p_{\mathrm{Re}} = f_{\mathrm{Pu}}(q_{\mathrm{Pu}}). \tag{2b}$$

In a junction Jc_i, $i = 1, ..., n_{\mathrm{Jc}}$, the amount of mass entering and leaving Jc_i is equal due to mass conservation. Summarizing the indices of pipes, pumps and demand branches that are incident to Jc_i in the set $\mathcal{E}_{inc}(\mathrm{Jc}_i)$, we thus get that

$$\sum_{j \in \mathcal{E}_{inc}(\mathrm{Jc}_i)} q_j = 0.$$

Using the incidence matrix, the sum of all mass flows entering or leaving a junction Jc_i is given by $e_i^T Aq = \sum_{j \in \mathcal{E}_{inc}(\mathrm{Jc}_i)} q_j$, such that the junction equations can be summarized as

$$A_{\mathrm{Jc,Pi}} q_{\mathrm{Pi}} + A_{\mathrm{Jc,Pu}} q_{\mathrm{Pu}} + A_{\mathrm{Jc,De}} q_{\mathrm{De}} = 0. \tag{2c}$$

In a demand branch De_i, $i = 1, ..., n_{\mathrm{De}}$, the mass flow q_{De_i} is specified on an interval $\mathcal{I}_{\mathrm{De}_i} \subset \mathbb{R}$ by a given function $\bar{q}_{\mathrm{De}_i} : \mathcal{I}_{\mathrm{De}_i} \to \mathbb{R}^{n_{\mathrm{De}}}$, i.e.,

$$q_i = \bar{q}_{\mathrm{De}_i}.$$

Similarly, in a reservoir Re_i, $i = 1, ..., n_{\mathrm{Re}}$, the pressure p_{Re_i} is specified on an interval $\mathcal{I}_{\mathrm{Re}_i} \subset \mathbb{R}$ by a function $\bar{p}_{\mathrm{Re}_i} : \mathcal{I}_{\mathrm{Re}_i} \to \mathbb{R}^{n_{\mathrm{Re}}}$, i.e.,

$$p_i = \bar{p}_{\mathrm{Re}_i}.$$

Setting $\bar{q}_{\mathrm{De}} := [q_{\mathrm{De}_j}]_{j=1,...,n_{\mathrm{De}}} : \mathcal{I}_{\mathrm{De}} \to \mathbb{R}^{n_{\mathrm{De}}}$ and $\bar{p}_{\mathrm{Re}} := [p_{\mathrm{Re}_i}]_{i=1,...,n_{\mathrm{Re}}} : \mathcal{I}_{\mathrm{Re}} \to \mathbb{R}^{n_{\mathrm{Re}}}$ with $\mathcal{I}_{\mathrm{De}} = \cap_{i=1,...,n_{\mathrm{De}}} \mathcal{I}_{\mathrm{De}_i}$ and $\mathcal{I}_{\mathrm{Re}} = \cap_{i=1,...,n_{\mathrm{Re}}} \mathcal{I}_{\mathrm{Re}_i}$, the boundary conditions are summarized as

$$q_{\mathrm{De}} = \bar{q}_{\mathrm{De}}, \tag{2d}$$
$$p_{\mathrm{Re}} = \bar{p}_{\mathrm{Re}}. \tag{2e}$$

In conclusion, the dynamics of the network $\mathcal{N}$ are modeled by the DAE (2) with unknowns $q(t)$ and $p(t)$.

3 Functional Mock-Up Units

A Functional Mock-Up Unit[10] (FMU) is represented as an input-output system of the form

$$\dot{x} = f_{\mathrm{St}}(t, x, u),$$
$$y = g_{\mathrm{out}}(t, x, u),$$

with state $x = [x_1, ..., x_{n_{\mathrm{St}}}]$, input $u = [u_1, ..., u_{n_u}]$ and output $y = [y_1, ..., y_{n_y}]$ related by the state and output function f_{St} and g_{out}, respectively. Constructed as a black-box model, the state and output function f_{St} and g_{out} are not known explicitly. Information about the entry pattern of the partial derivatives, however, is given in the form of

$$[g_{\mathrm{out},u}]_{ij} = \begin{cases} 0, & \text{if output } g_{\mathrm{out},i} \text{ is independent of input } u_j, \\ \textit{constant}, & \text{if output } g_{\mathrm{out},i} \text{ depends linearly on input } u_j, \\ \neq 0, & \text{if output } g_{\mathrm{out},i} \text{ depends on input } u_j, \end{cases}$$

where $g_{\mathrm{out},u}$ denotes the partial derivatives of the output function g_{out} with respect to the input u and $[g_{\mathrm{out},u}]_{ij}$ denotes its components for $i = 1, ..., n_y$ and $j = 1, ..., n_u$. The same information is available for $g_{\mathrm{out},x}$, $f_{\mathrm{St},u}$ and $f_{\mathrm{St},x}$.

We consider FMUs having one scalar input $u \in \mathbb{R}$ and one scalar output $y \in \mathbb{R}$. The state x, however, might be of higher dimension. Furthermore, we distinguish between *demand FMUs* $\mathcal{B}_{\mathrm{De}}$ whose outputs are mass flows while the inputs are pressures, and *reservoir FMUs* $\mathcal{B}_{\mathrm{Re}}$ whose outputs are pressures while the inputs are mass flows. The reservoir FMUs are further partitioned into *pipe*

[10] http://fmi-standard.org/

reservoir FMUs $\mathcal{B}_{\mathrm{Re,Pi}}$ whose inputs are mass flows from pipes, and *pump reservoir FMUs* $\mathcal{B}_{\mathrm{Re,Pu}}$ whose inputs are mass flows from pumps.

Given a collection of n_{De_c} demand FMUs $\mathcal{B}_{\mathrm{De}_1}, ..., \mathcal{B}_{\mathrm{De}_{n_{\mathrm{De}_c}}}$, we summarize the state and output functions as $f_{\mathrm{De}} = [f_{\mathrm{St,De}_1}, ..., f_{\mathrm{St,De}_{n_{\mathrm{De}_c}}}]$, $g_{\mathrm{De}} = [g_{\mathrm{out,De}_1}, ..., g_{\mathrm{out,De}_{n_{\mathrm{De}_c}}}]$, the in- and outputs as $u_{\mathrm{De}} = [u_{\mathrm{De}_1}, ..., u_{\mathrm{De}_{n_{\mathrm{De}_c}}}]$, $y_{\mathrm{De}} = [y_{\mathrm{De}_1}, ..., y_{\mathrm{De}_{n_{\mathrm{De}_c}}}]$ and the states as $x_{\mathrm{De}} = [x_{\mathrm{De}_1}, ..., x_{\mathrm{De}_{n_{\mathrm{De}_c}}}]$. Then, the state and output equations of the demand FMUs are summarized as

$$\dot{x}_{\mathrm{De}} = f_{\mathrm{De}}(t, x_{\mathrm{De}}, u_{\mathrm{De}}), \tag{3a}$$

$$y_{\mathrm{De}} = g_{\mathrm{De}}(t, x_{\mathrm{De}}, u_{\mathrm{De}}). \tag{3b}$$

In the same manner, given a collection of of n_{Re_c} pipe or pump reservoir FMUs $\mathcal{B}_{\mathrm{Re}_1,P}, ..., \mathcal{B}_{\mathrm{Re}_{n_{\mathrm{Re}_c}},P}$, we summarize the state and output functions as $f_{\mathrm{Re},P} = [f_{\mathrm{St,Re}_1,P}, ..., f_{\mathrm{St,Re}_{n_{\mathrm{Re}_c}},P}]$ and $g_{\mathrm{Re},P} = [g_{\mathrm{out,Re}_1,P}, ..., g_{\mathrm{out,Re}_{n_{\mathrm{Re}_c}},P}]$, the in- and outputs as $u_{\mathrm{Re},P} = [u_{\mathrm{Re}_1,P}, ..., u_{\mathrm{Re}_{n_{\mathrm{Re}_c}},P}]$ and $y_{\mathrm{Re},P} = [y_{\mathrm{Re}_1,P}, ..., y_{\mathrm{Re}_{n_{\mathrm{Re}_c}},P}]$ and the states as $x_{\mathrm{Re},P} = [x_{\mathrm{Re}_1,P}, ..., x_{\mathrm{Re}_{n_{\mathrm{Re}_c}},P}]$ for $P \in \{\mathrm{Pi}, \mathrm{Pu}\}$. The state and output equations then read

$$\dot{x}_{\mathrm{Re},P} = f_{\mathrm{Re},P}(t, x_{\mathrm{Re},P}, u_{\mathrm{Re},P}), \tag{3c}$$

$$y_{\mathrm{Re},P} = g_{\mathrm{Re},P}(t, x_{\mathrm{Re},P}, u_{\mathrm{Re},P}) \tag{3d}$$

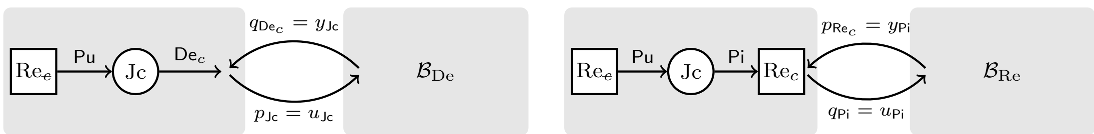
for $P \in \{\mathrm{Pi}, \mathrm{Pu}\}$. For our analysis, we assume that the state and output functions are defined on the set $\mathcal{I}_\star \times \mathbb{R}^{n_{\mathrm{St},\star_c}} \times \Omega_{\star_c}$ for $\star \in \{\mathrm{De}, (\mathrm{Re}, \mathrm{Pi}), (\mathrm{Re}, \mathrm{Pu})\}$, where $n_{\mathrm{St},\star_c}$ denotes the number of respective states, $\mathcal{I}_\star \subset \mathbb{R}$ and $\Omega_{\star_c} \in \mathbb{R}^{n_{\star_c}}$.

Regarding the dependency of the input, we make the following definition.

Definition 1 *We call a FMU $\mathcal{B}$ with state function f_{St} and output function g_{out} input independent, if $f_{St,u} = 0$ and $g_{out,u} = 0$.*

Note that it is not sufficient that the output function is independent of the input u, as the state x may still depend on u via the state function.

4 Coupling of networks and FMUs



(a) Example of coupling a demand FMU $\mathcal{B}_{\mathrm{De}}$. (b) Example of coupling a reservoir FMU $\mathcal{B}_{\mathrm{Re}}$.

Fig. 2: Coupling a network $\mathcal{N}$ with demand and reservoir FMUs.

Now, we consider the coupling of a collection of FMUs to a network $\mathcal{N}$, which is performed via the boundary conditions $\mathcal{DE}$ and $\mathcal{RE}$. Given a collection of demand FMUs $\mathcal{B}_{\mathrm{De}_1}, ..., \mathcal{B}_{\mathrm{De}_{n_{\mathrm{De}_c}}}$ and pipe and pump reservoir FMUs $\mathcal{B}_{\mathrm{Re}_1,P}, ..., \mathcal{B}_{\mathrm{Re}_{n_{\mathrm{Re}_c}},P}$, $P \in \{\mathrm{Pi}, \mathrm{Pu}\}$, the boundary conditions are partitioned into those coupled to the demand and reservoir FMUs and those connected to a given input function $\bar{q}_{\mathrm{De}}$ and $\bar{p}_{\mathrm{Re}}$. The first ones, the *coupling boundary conditions*, are denoted by $\mathrm{De}_{c,1}, ..., \mathrm{De}_{c,n_{\mathrm{De}_c}}$ and $\mathrm{Re}_{c,1}, ..., \mathrm{Re}_{c,n_{\mathrm{Re}_c}}$, respectively. The latter ones, the *non-coupling boundary conditions*, are denoted by $\mathrm{De}_{e,1}, ..., \mathrm{De}_{e,n_{\mathrm{De}_e}}$ and $\mathrm{Re}_{e,1}, ..., \mathrm{Re}_{e,n_{\mathrm{Re}_e}}$, respectively. The elements adjacent to the coupling boundary conditions are called *coupling elements* and are denoted by $\mathrm{Jc}_{c,1}, ..., \mathrm{Jc}_{c,n_{\mathrm{De}_c}}$ and $P_{c,1}, ..., P_{c,n_{\mathrm{Re}_c}}$, $P \in \{\mathrm{Pi}, \mathrm{Pu}\}$. By Assumption 1*(4)*, there exists a numbering such that every boundary condition

$\mathrm{De}_{c,i}$ or $\mathrm{Re}_{c,i}$ is connected to the element Jc_i or P_i, $P \in \{\mathrm{Pi}, \mathrm{Pu}\}$, as well as to the demand or reservoir FMU $\mathcal{B}_{\mathrm{De}_i}$ or $\mathcal{B}_{\mathrm{Re}_i,P}$, respectively.

The coupling of the FMUs to the network $\mathcal{N}$ is performed by identifying the in- and outputs of the FMUs with the respective coupling elements and boundary conditions. For the demand FMUs $\mathcal{B}_{\mathrm{De}_1}, ..., \mathcal{B}_{\mathrm{De}_{n_{\mathrm{De}_c}}}$, this results in adding the equations

$$q_{\mathrm{De}_c} = y_{\mathrm{De}}, \tag{4a}$$
$$p_{\mathrm{Jc}_c} = u_{\mathrm{De}}, \tag{4b}$$

i.e., the coupling demand flows q_{De_c} are identified with the outputs y_{De} while the pressure s p_{Jc_c} in the coupling junctions serve as inputs u_{De}, cf. Figure 2a. For the reservoir FMUs $\mathcal{B}_{\mathrm{Re}_1,P}, ..., \mathcal{B}_{\mathrm{Re}_{n_{\mathrm{Re}_c}},P}$ the coupling is performed by adding the equations

$$p_{\mathrm{Re}_c} = y_{\mathrm{Re},P}, \tag{4c}$$
$$q_{P_c} = u_{\mathrm{Re},P}, \;\; P \in \{\mathrm{Pi}, \mathrm{Pu}\}, \tag{4d}$$

i.e., the coupling reservoir pressures p_{Re_c} are identified with the outputs $y_{\mathrm{Re},P}$ while the mass flows q_{P_c} of the coupling pipes or pumps serve as input $u_{\mathrm{Re},P}$, cf. Figure 2b.

In the following, we summarize the states of demand and reservoir FMUs as $x = [x_{\mathrm{De}}^T, x_{\mathrm{Re,Pi}}^T, x_{\mathrm{Re,Pu}}^T]^T$ and the state functions as $f_{\mathrm{St}} = [f_{\mathrm{De}}^T, f_{\mathrm{Re,Pi}}^T, f_{\mathrm{Re,Pu}}^T]^T$.

In conclusion, the dynamics of the network $\mathcal{N}$ coupled to FMUs are modeled by the DAE (2), the FMU equations (3) and the coupling conditions (4). To analyze the solvability of this coupled system, we define the network function

$$F := \left[F_{\mathcal{B}_{\mathrm{St}}}^T, F_{\mathrm{Pi}}^T, F_{\mathrm{Pu}}^T, F_{\mathrm{Jc}}^T, F_{\mathcal{B}_{\mathrm{De}}}^T, F_{\mathcal{B}_{\mathrm{Re,Pi}}}^T, F_{\mathcal{B}_{\mathrm{Re,Pu}}}^T\right]^T, \tag{5}$$

where the component functions are defined by

$$F_{\mathcal{B}_{\mathrm{St}}} := \dot{x} - f_{\mathrm{St}}(t, x, p_{\mathrm{Jc}_c}, q_{\mathrm{Pi}_c}, q_{\mathrm{Pu}_c}) \tag{6a}$$
$$F_{\mathrm{Pi}} := \dot{q}_{\mathrm{Pi}} - f_{\mathrm{Pi}}(q_{\mathrm{Pi}}, p_{\mathrm{Jc}}, y_{\mathrm{Re,Pi}}, \bar{p}_{\mathrm{Re}}) \tag{6b}$$
$$F_{\mathrm{Pu}} := A_{\mathrm{Jc,Pu}}^T p_{\mathrm{Jc}} + A_{\mathrm{Re}_e,\mathrm{Pu}_e}^T \bar{p}_{\mathrm{Re}_e} + y_{\mathrm{Re,Pu}} - f_{\mathrm{Pu}}(q_{\mathrm{Pu}}) \tag{6c}$$
$$F_{\mathrm{Jc}} := A_{\mathrm{Jc,Pi}} q_{\mathrm{Pi}} + A_{\mathrm{Jc,Pu}} q_{\mathrm{Pu}} + y_{\mathrm{De}} + A_{\mathrm{Jc}_e,\mathrm{De}} \bar{q}_{\mathrm{De}} \tag{6d}$$
$$F_{\mathcal{B}_{\mathrm{De}}} := y_{\mathrm{De}} - g_{\mathrm{De}}(t, x, p_{\mathrm{Jc}_c}) \tag{6e}$$
$$F_{\mathcal{B}_{\mathrm{Re,Pi}}} := y_{\mathrm{Re,Pi}} - g_{\mathrm{Re,Pi}}(t, x, q_{\mathrm{Pi}_c}) \tag{6f}$$
$$F_{\mathcal{B}_{\mathrm{Re,Pu}}} := y_{\mathrm{Re,Pu}} - g_{\mathrm{Re,Pu}}(t, x, q_{\mathrm{Pu}_c}). \tag{6g}$$

In (6) we have already inserted the boundary and coupling conditions (2d), (2e) and (4) in (2a)-(2c). The function arguments of (5) are summarized as

$$X := \left[x^T, q_{\mathrm{Pi}}^T, q_{\mathrm{Pu}}^T, p_{\mathrm{Jc}}^T, y_{\mathrm{De}}^T, y_{\mathrm{Re,Pi}}^T, y_{\mathrm{Re,Pu}}^T\right]^T.$$

Then, the dynamics of the coupled system are modeled by the DAE

$$F(X) = 0. \tag{7}$$

The system is square with dimension $n = n_{\mathrm{St}} + n_{\mathrm{Pi}} + n_{\mathrm{Pu}} + n_{\mathrm{Jc}} + n_{\mathrm{De}_c} + n_{\mathrm{Re}_c}$. The number of differential and algebraic equations in (7) is given by

$$d := n_{\mathrm{St}} + n_{\mathrm{Pi}} \tag{8a}$$
$$a := n_{\mathrm{De}_c} + n_{\mathrm{Re}_c} + n_{\mathrm{Jc}} + n_{\mathrm{Pu}}. \tag{8b}$$

For the ease of notation, we summarize the differential and algebraic equations by

$$\begin{aligned} F_d &:= [F_{\mathcal{B}_{\mathrm{St}}}^T, F_{\mathrm{Pi}}^T]^T, \\ F_a &:= [F_{\mathrm{Pu}}^T, F_{\mathrm{Jc}}^T, F_{\mathcal{B}_{\mathrm{De}}}^T, F_{\mathcal{B}_{\mathrm{Re,Pi}}}^T, F_{\mathcal{B}_{\mathrm{Re,Pu}}}^T]^T, \end{aligned}$$

and the differential and algebraic variables by

$$\begin{aligned} X_d &:= [x^T, q_{\mathrm{Pi}}^T]^T, \\ X_a &:= [q_{\mathrm{Pu}}^T, p_{\mathrm{Jc}}^T, y_{\mathrm{De}}^T, y_{\mathrm{Re,Pi}}^T, y_{\mathrm{Re,Pu}}^T]^T. \end{aligned}$$

5 Graph theoretical prerequisites

To characterize the solvability of the DAE (7), we introduce the relevant substructures of the network $\mathcal{N}$. Therefore, we use graph theoretical concepts like paths, spanning trees, cycles, connected components, etc. A comprehensive introduction to this topic can be found, e.g., in [4,6,20]. For our purposes, however, we need these concepts for subsets describing the connection structure of two specific element types, like e.g. the junction and pump subset $\mathcal{G}_{\mathrm{Jc,Pu}} := \{\mathcal{JC}, \mathcal{PU}\}$. Still, the ideas of trees, cycles, etc. and their correspondence to fundamental subspaces of the connection matrix can be easily extended, see [2].

First, we consider the subset of junctions and pumps $\{\mathrm{Jc}, \mathrm{Pu}\}$. This set is composed of $n_{\mathcal{C}}$ maximally connected components $\mathcal{C}_1, ..., \mathcal{C}_{n_{\mathcal{C}}}$, i.e., in each set $\mathcal{C}_I$ every pair of junctions is connected by a path of pumps, whereas there is no such pump connection between the junctions of two different components $\mathcal{C}_I$, $\mathcal{C}_J$, $I \neq J$. Hence, $\{\mathrm{Jc}, \mathrm{Pu}\} = \bigcup_{I=1}^{n_{\mathcal{C}}} \mathcal{C}_I$ with $\mathcal{C}_I \cap \mathcal{C}_J = \emptyset$, $I \neq J$. According to their connection to reservoirs, the maximally connected components are partitioned into $n_{\mathcal{C}_{\mathrm{Re}}}$ components *with* a connection to a reservoir or reservoir FMU, i.e.,

$$\mathcal{C}_{\mathrm{Re}} := \{\mathcal{C}_I \in \mathcal{G}_{\mathrm{Jc,Pu}} |\ \exists\ \mathrm{Jc}_{i_1}, \mathrm{Pu}_i \in \mathcal{C}_I,\ \mathrm{Re}_{i_2} \in \mathcal{RE} \colon \mathrm{Pu}_i = (\mathrm{Jc}_{i_1}, \mathrm{Re}_{i_2})\}$$

and $n_{\mathcal{C}_{\cancel{\mathrm{Re}}}}$ components *without* a connection to a reservoir or reservoir FMU, i.e.,

$$\mathcal{C}_{\cancel{\mathrm{Re}}} := \{\mathcal{C}_I \in \mathcal{G}_{\mathrm{Jc,Pu}} |\ \forall\ \mathrm{Pu}_i \in \mathcal{C}_I \exists\ \mathrm{Jc}_{i_1}, \mathrm{Jc}_{i_2} \in \mathcal{C}_I \colon \mathrm{Pu}_i = (\mathrm{Jc}_{i_1}, \mathrm{Jc}_{i_2})\}.$$

Note that junctions connected to pipes only are *isolated* in $\{\mathrm{Jc}, \mathrm{Pu}\}$, i.e., correspond to components in $\mathcal{C}_{\cancel{\mathrm{Re}}}$. The components $\mathcal{C}_{\cancel{\mathrm{Re}}}$ are further partitioned with respect to the coupled demand FMUs. Pump components without a reservoir but with at least one demand FMU depending on its input pressure are called *FMU dependent* components and are denoted by

$$\mathcal{C}_{\cancel{\mathrm{Re}},\mathcal{B}_{\mathrm{De}}} := \{\mathcal{C}_I \in \mathcal{C}_{\cancel{\mathrm{Re}}} \mid \mathcal{C}_I \cap \mathcal{JC}_c \neq \emptyset,\ \exists\ \mathrm{Jc}_c \in \mathcal{C}_I \colon f_{\mathrm{De},p_{\mathrm{Jc}_c}} \cdot g_{\mathrm{De},p_{\mathrm{Jc}_c}} \neq 0\}. \tag{9}$$

Pump components without a reservoir containing only demand FMUs independent of the input pressure or containing no demand FMU at all are called *hidden constraint* (HC) components and are denoted by

$$\begin{aligned} \mathcal{C}_{\cancel{\mathrm{Re}},\mathrm{HC}} := \{\mathcal{C}_I \in \mathcal{C}_{\cancel{\mathrm{Re}}} \mid\ & \mathcal{C}_I \cap \mathcal{JC}_c = \emptyset \text{ or} \\ & \mathcal{C}_I \cap \mathcal{JC}_c \neq \emptyset,\ \forall\ \mathrm{Jc}_c \in \mathcal{C}_I \colon f_{\mathrm{De},p_{\mathrm{Jc}_c}} = 0,\ g_{\mathrm{De},p_{\mathrm{Jc}_c}} = 0\}. \end{aligned} \tag{10}$$

We set $n_{\mathcal{B}_{\mathrm{De}}} := |\mathcal{C}_{\cancel{\mathrm{Re}},\mathcal{B}_{\mathrm{De}}}|$ and $n_{\mathrm{HC}} := |\mathcal{C}_{\cancel{\mathrm{Re}},\mathrm{HC}}|$.

In a connected pump component containing a reservoir, the pressure in every junction is well defined. In a connected pump component without connection to a reservoir, only the pressure *difference* is specified. To specify the *absolute* pressure in the junctions of these components, a reference junction has to be appointed, whose pressure is specified by an additional condition. In the hidden constraint components $\mathcal{C}_{\cancel{\mathrm{Re}},\mathrm{HC}}$, this additional condition is given by an algebraic equation arising from the mass balance. In the FMU dependent components $\mathcal{C}_{\cancel{\mathrm{Re}},\mathcal{B}_{\mathrm{De}}}$, the additional condition is obtained from the input-output relation of the FMU.

Hence, for every component $\mathcal{C}_I \in \mathcal{C}_{\cancel{\mathrm{Re}}}$, we designate a reference junction $\mathrm{Jc}_{\mathrm{ref},I}$ and refer to its pressure as $p_{\mathrm{Jc}_{\mathrm{ref}},I}$. We write $p_{\mathrm{Jc}_{\mathrm{ref}},\mathrm{HC},I}$ if $\mathcal{C}_I \in \mathcal{C}_{\cancel{\mathrm{Re}},\mathrm{HC}}$ and $p_{\mathrm{Jc}_{\mathrm{ref}},\mathcal{B}_{\mathrm{De}},I}$ if $\mathcal{C}_I \in \mathcal{C}_{\cancel{\mathrm{Re}},\mathcal{B}_{\mathrm{De}}}$. The remaining non-reference junctions are referred as $\mathcal{JC}_{\cancel{\mathrm{ref}},I}$ and the pressure difference between these non-reference junctions and the reference junction is denoted by $p_{\mathrm{Jc}_{\mathrm{diff}},I}$.

For a component $\mathcal{C}_I \in \mathcal{C}_{\mathrm{Re}}$, no reference junction needs to be chosen as it is already given by the reservoir. Thus, all junctions of $\mathcal{C}_I$ are non-reference junctions and the pressure in each junction is well-defined. For a uniform notation, however, we denote the pressures of these components also by $p_{\mathrm{Jc}_{\mathrm{diff}},I}$.

Algebraically, these pressures are obtained from the variable transformation

$$\Pi_{p_{\mathrm{Jc}}} := \left[\Pi_{p_{\mathrm{diff}}}\ \Pi_{p_{\mathrm{ref}},\mathcal{B}_{\mathrm{De}}}\ \Pi_{p_{\mathrm{ref}},\mathrm{HC}}\right], \tag{11}$$

where $\Pi_{p_{\mathrm{diff}}} := \mathrm{diag}(\Pi_{p_{\mathrm{diff}},I})_{\mathcal{C}_I\in\mathcal{C}}$ and $\Pi_{p_{\mathrm{ref}},\star} := \mathrm{diag}(\Pi_{p_{\mathrm{ref}},\star,I})_{\mathcal{C}_I\in\mathcal{C}_{\cancel{\mathrm{Re}},\star}}$, $\star \in \{\mathcal{B}_{\mathrm{De}}, \mathrm{HC}\}$ are given by

$$\begin{aligned}
\Pi_{p_{\mathrm{diff}},I} &:= \begin{cases} \Pi_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},I}, & \mathcal{C}_I \in \mathcal{C}_{\mathrm{Re}}, \\ \left(\Pi^T_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},I}(\Pi_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},I}\Pi^T_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},I} - (\mathbf{1}_I - e_{\mathrm{Jc}_{\mathrm{ref}},I})e^T_{\mathrm{Jc}_{\mathrm{ref}},I})\right)^T, & \mathcal{C}_I \in \mathcal{C}_{\cancel{\mathrm{Re}}}, \end{cases} \\
\Pi_{p_{\mathrm{ref}},\mathcal{B}_{\mathrm{De}},I} &:= e_{\mathrm{Jc}_{\mathrm{ref}},I}, \qquad \mathcal{C}_I \in \mathcal{C}_{\cancel{\mathrm{Re}},\mathcal{B}_{\mathrm{De}}}, \\
\Pi_{p_{\mathrm{ref}},\mathrm{HC},I} &:= e_{\mathrm{Jc}_{\mathrm{ref}},I}, \qquad \mathcal{C}_I \in \mathcal{C}_{\cancel{\mathrm{Re}},\mathrm{HC}}.
\end{aligned}$$

The matrix $\Pi_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},I} := [e_i]_{\mathrm{Jc}_i\in\mathcal{JC}_{\cancel{\mathrm{ref}}}}$ selects the non-reference junctions using the standard canonical basis vectors $e_i \in \mathbb{R}^{n_{\mathrm{Jc}_I}}$, $n_{\mathrm{Jc}_I} := |\{\mathrm{Jc}_i \in \mathcal{C}_I\}|$, $e_{\mathrm{Jc}_{\mathrm{ref}},I} \in \mathbb{R}^{n_{\mathrm{Jc}_I}}$ selects the reference junction $\mathrm{Jc}_{\mathrm{ref},I}$ and $\mathbf{1}_I = [1,...,1]^T \in \mathbb{R}^{n_{\mathrm{Jc}_I}}$.

The associated variables are denoted by

$$\begin{aligned}
p_{\mathrm{diff}} &:= \Pi^T_{p_{\mathrm{diff}}} p_{\mathrm{Jc}}, \\
p_{\mathcal{B}_{\mathrm{De}}} &:= \Pi^T_{p_{\mathrm{ref}},\mathcal{B}_{\mathrm{De}}} p_{\mathrm{Jc}}, \\
p_{\mathrm{HC}} &:= \Pi^T_{p_{\mathrm{ref}},\mathrm{HC}} p_{\mathrm{Jc}}.
\end{aligned}$$

For the equations, we select all non-reference junctions in the network using the matrix $\Pi_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}}$. For the components without a reservoir, we consider the *vertex identification*, merging all junction of such a component in a supernode, i.e., we set

$$\overline{\mathrm{Jc}}_{i,I} := \bigcup_{\mathrm{Jc}_j\in\mathcal{C}_I} \mathrm{Jc}_j, \quad \mathcal{C}_I \in \mathcal{C}_{\cancel{\mathrm{Re}},i},\ i \in \{\mathcal{B}_{\mathrm{De}}, \mathrm{HC}\}.$$

Algebraically, the vertex identification of a component $\mathcal{C}_I$ is performed using the vector $\mathbf{1}_I = [1,...,1]^T \in \mathbb{R}^{n_{\mathrm{Jc}_I}}$. Setting

$$\begin{aligned}
\Pi_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}} &:= \mathrm{diag}(\Pi_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},I})_{\mathcal{C}_I\in\mathcal{C}}, \\
\Pi_{\mathcal{B}_{\mathrm{De}}} &:= \mathrm{diag}(\mathbf{1}_I)_{\mathcal{C}_I\in\mathcal{C}_{\cancel{\mathrm{Re}},\mathcal{B}_{\mathrm{De}}}}, \\
\Pi_{\mathrm{HC}} &:= \mathrm{diag}(\mathbf{1}_I)_{\mathcal{C}_I\in\mathcal{C}_{\cancel{\mathrm{Re}},\mathrm{HC}}},
\end{aligned}$$

we construct our equation transformation as

$$\Pi_{F_{\mathrm{Jc}}} := \left[\Pi_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}}\ \Pi_{\mathcal{B}_{\mathrm{De}}}\ \Pi_{\mathrm{HC}}\right]. \tag{12}$$

The associated network functions are denoted by

$$\begin{aligned}
F_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}} &:= \Pi^T_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}} F_{\mathrm{Jc}} \\
F_{\overline{\mathrm{Jc}}_{\mathcal{B}\mathrm{De}}} &:= \Pi^T_{\mathcal{B}_{\mathrm{De}}} F_{\mathrm{Jc}}, \\
F_{\overline{\mathrm{Jc}}_{\mathrm{HC}}} &:= \Pi^T_{\mathrm{HC}} F_{\mathrm{Jc}}.
\end{aligned}$$

The function $F_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}}$ comprises the mass balances of the non-reference junctions in the network. The functions $F_{\mathcal{B}_{\mathrm{De}}}$, F_{HC} sum up the mass balances of every component without a reservoir.

The matrix $\Pi_{F_{\mathrm{Jc}}}$ filters out the FMU dependent and hidden constraint components of the incidence matrix $A_{\mathrm{Jc},\mathrm{Pu}}$ and inverts the variable transformation $\Pi_{p_{\mathrm{Jc}}}$.

Lemma 1 *[2] Consider $\Pi_{p_{Jc}}$ and $\Pi_{F_{Jc}}$ as defined in* (11) *and* (12). *Then, the following statements are valid:*

1. $\Pi_{p_{Jc}}^T \Pi_{F_{Jc}} = \Pi_{F_{Jc}}^T \Pi_{p_{Jc}} = I_{n_{Jc}}$.
2. $\operatorname{span}(\Pi_{Jc_{\cancel{ref}}}) = \operatorname{corange}(A_{Jc,Pu})$ *and* $\operatorname{span}([\Pi_{\mathcal{B}_{De}}, \Pi_{HC}]) = \operatorname{coker}(A_{Jc,Pu})$.

Let $\Pi_{i,c}$, denote the rows of Π_i, $i \in \{\mathrm{Jc}_{\cancel{\mathrm{ref}}}, \mathcal{B}_{\mathrm{De}}, \mathrm{HC}\}$, selecting or summing only the coupling junctions, respectively. For referring to a particular component $\mathcal{C}_I$, the notation $\Pi_{i,c,I}$ is used. For the Jacobian $g_{\mathrm{De},p_{\mathrm{Jc}_c},I}$ of the output function g_{De} of the demand FMUs with respect to its input pressure p_{Jc_c} associated with a component $\mathcal{C}_I$, we set

$$\begin{aligned} G_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}} &:= \Pi_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},c}^T g_{\mathrm{De},p_{\mathrm{Jc}_c}} \Pi_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},c}, \\ G_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathcal{B}_{\mathrm{De}}} &:= \Pi_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},c}^T g_{\mathrm{De},p_{\mathrm{Jc}_c}} \Pi_{\mathcal{B}_{\mathrm{De}},c}, \\ G_{\mathcal{B}_{\mathrm{De}}} &:= \Pi_{\mathcal{B}_{\mathrm{De}},c}^T g_{\mathrm{De},p_{\mathrm{Jc}_c}} \Pi_{\mathcal{B}_{\mathrm{De}},c}. \end{aligned} \tag{13}$$

Note that

$$\begin{aligned} G_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathrm{HC}} &:= \Pi_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},c}^T g_{\mathrm{De},p_{\mathrm{Jc}_c}} \Pi_{\mathrm{HC},c}, \\ G_{\mathrm{HC}} &:= \Pi_{\mathrm{HC},c}^T g_{\mathrm{De},p_{\mathrm{Jc}_c}} \Pi_{\mathrm{HC},c}, \end{aligned}$$

all vanish by the definition of $\mathcal{C}_{\cancel{\mathrm{Re}},\mathrm{HC}}$.

Assumption 2 *Consider a network $\mathcal{N}$ as in* (1). *One of the following conditions is satisfied.*

(i) There are no input-dependent demand FMUs, i.e., $\mathcal{C}_{\cancel{Re},\mathcal{B}_{De}} = \emptyset$.
(ii) If there are input-dependent demand FMUs, i.e., if $\mathcal{C}_{\cancel{Re},\mathcal{B}_{De}} \neq \emptyset$, then every $\mathcal{C}_I \in \mathcal{C}_{\cancel{Re},\mathcal{B}_{De}}$ contains exactly one demand FMU depending on the pressure input and the associated coupling junction is chosen as reference junction of the component.

Given Assumption 2, we specify the rank of the matrices given in (13).

Lemma 2 *Consider the matrices as defined in* (13). *If and only if Assumption 2 is satisfied, then $G_{Jc_{\cancel{ref}}} = 0$, $G_{Jc_{\cancel{ref}},\mathcal{B}_{De}} = 0$ and $G_{\mathcal{B}_{De}}$ is non-singular with* $\operatorname{rank}(G_{\mathcal{B}_{De}}) = n_{\mathcal{B}_{De}}$.

Proof As every FMU $\mathcal{B}_k$ only depends on the input p_{Jc_j} of its own coupling junction Jc_j, the Jacobian $g_{\mathrm{De},p_{\mathrm{Jc}_c}}$ is diagonal. In combination with the structure of $\Pi_{F_{\mathrm{Jc}}}$, we have that

$$G_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}} = \operatorname{diag}(g_{\mathrm{De}_j,p_{\mathrm{Jc}_j}})_{\mathrm{Jc}_j \in \mathcal{JC}_{\cancel{\mathrm{ref}},I}, I=1,\dots,n_{\mathcal{C}}}, \tag{14a}$$

$$G_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathcal{B}_{\mathrm{De}}} = [g_{\mathrm{De}_j,p_{\mathrm{Jc}_j}}]_{\mathrm{Jc}_j \in \mathcal{JC}_{\cancel{\mathrm{ref}},I}, I=1,\dots,n_{\mathcal{C}}}, \tag{14b}$$

$$G_{\mathcal{B}_{\mathrm{De}}} = \operatorname{diag}\Big(\sum_{\mathrm{Jc}_{\mathrm{ref,I}} \in \mathcal{C}_I} g_{\mathrm{De}_{\mathrm{ref,I}},p_{\mathrm{Jc}_{\mathrm{ref,I}}}}\Big)_{I=1,\dots,n_{\mathcal{C}}}. \tag{14c}$$

If Assumption 2 is satisfied, then $G_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}} = 0$, $G_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathcal{B}_{\mathrm{De}}} = 0$ and $G_{\mathcal{B}_{\mathrm{De}}} \neq 0$. This follows immediately from the structure of the matrices given in (14). □

Now, we turn to the pump flows of the connected components. For each pump component $\mathcal{C}_I$, we choose a spanning tree $\mathcal{PU}_{\mathrm{tree,I}}$, which is a choice of a largest subgraph of $\{\mathrm{Jc}, \mathrm{Pu}\}$ without cycles and without paths between reservoirs, reservoir FMUs or reservoirs and reservoir FMUs. Pumps that either close a cycle or a path between reservoirs or reservoir FMUs are called *chords* and are summarized in the chord set $\mathcal{PU}_{\mathrm{chord},I}$. This definition naturally extends the definition of a spanning tree and its chord set made in [2]. We summarize the trees and their chord sets in the sets $\mathcal{PU}_{\mathrm{tree}} = \cup_{I=1,\dots,n_{\mathcal{C}}} \mathcal{PU}_{\mathrm{tree},I}$ and $\mathcal{PU}_{\mathrm{chord}} = \cup_{I=1,\dots,n_{\mathcal{C}}} \mathcal{PU}_{\mathrm{chord},I}$. The cycles and reservoir paths closed by the chords are called *closed pump paths*. For each chord $\mathrm{Pu}_\iota \in \mathcal{PU}_{\mathrm{chord}}$, we summarize the pumps lying on the cycle or path between reservoirs or reservoir FMUs closed by Pu_ι in the set

$$\mathcal{P}_{\mathrm{cl},\iota} := \big\{\mathrm{Pu}_i \in \mathcal{PU}_{\mathrm{tree}} \mid \mathrm{Pu}_i \text{ lies on the closed pump path defined by } \mathrm{Pu}_\iota\}.$$

The set of closed paths is denoted by $\mathcal{P}_{\rm cl} := \{\mathcal{P}_{{\rm cl},\iota} | {\rm Pu}_\iota \in \mathcal{PU}_{\rm chord}\}$. Given the Jacobians $f_{{\rm Pu},q_{\rm Pu}}$, $g_{{\rm Re,Pu},q_{{\rm Pu}_c}}$ of the pump function $F_{\rm Pu}$ and the output function of the reservoir FMUs $g_{\rm Re,Pu}$ with respect to the pump flow $q_{\rm Pu}$ and coupling pump flow $q_{{\rm Pu}_c}$, respectively, we define the matrix

$$D := \operatorname{diag}\left(0, g_{{\rm Re,Pu},q_{{\rm Pu}_c}}\right) - f_{{\rm Pu},q_{\rm Pu}}. \tag{15}$$

As every pump only depends on its own flow and every FMU depends only on its own input, the matrix D is diagonal. Closed pump paths satisfying

$$\mathcal{P}_{\rm cl,reg} := \left\{ \mathcal{P}_{{\rm cl},\iota} \in \mathcal{P}_{\rm cl} \mid D_{{\rm Pu}_\iota,{\rm Pu}_\iota} + \sum_{{\rm Pu}_i \in \mathcal{P}_{{\rm cl},\iota}} D_{{\rm Pu}_i,{\rm Pu}_i} \neq 0 \right\} \tag{16}$$

are called *regular* closed paths, where $D_{{\rm Pu}_i,{\rm Pu}_i}$ refers to the entry of D associated with ${\rm Pu}_i$. Closed pump paths satisfying

$$\mathcal{P}_{\rm cl,sgl} := \left\{ \mathcal{P}_{{\rm cl},\iota} \in \mathcal{P}_{\rm cl} \mid D_{{\rm Pu}_\iota,{\rm Pu}_\iota} + \sum_{{\rm Pu}_i \in \mathcal{P}_{{\rm cl},\iota}} D_{{\rm Pu}_i,{\rm Pu}_i} = 0 \right\} \tag{17}$$

are called *singular* pump paths. On singular pump paths, neither the pump flow nor the pressure is specified, hence we make the following assumption.

Assumption 3 *Consider a network $\mathcal{N}$ as in* (1).

(1) There is at least one reservoir or reservoir FMU, i.e., $n_{Re} > 0$.
(2) One of the following conditions is satisfied.
   (i) There are no closed pump paths in the network, i.e., $\mathcal{PU}_{chord} = \emptyset$.
   (ii) If there are closed pump paths in the network, i.e., if $\mathcal{PU}_{chord} \neq \emptyset$, then every closed path is regular, i.e., $\mathcal{P}_{cl} = \mathcal{P}_{cl,reg}$.

On the spanning tree $\mathcal{PU}_{\rm tree}$, the pressure difference is well defined by the pumps on $\mathcal{PU}_{s,\rm tree}$. On closed pump paths, however, the pressure difference is fixed externally. On cycles of pumps, the pressure difference vanishes as the path is closed, while on paths of pumps between reservoirs and/or reservoir FMUs, the pressure drop across the path is fixed by these components. Hence, on these substructures at least one pump has to work against its usual mode of operation: instead of returning a pressure drop for a given mass flow, it has to adjust the mass flow to a given pressure. This means that the pump characteristic has to be invertible. Choosing this pump as reference pump, the differences of the pump flows on the closed path with respect to the reference pump are specified by the mass balance.

To identify these mass flows, we construct a suitable variable transformation. Naturally, we choose the chords as reference pumps of the associated closed path. For a component $\mathcal{C}_I$, the chords ${\rm Pu}_\iota \in \mathcal{PU}_{{\rm chord},I}$ are selected by

$$\Pi_{{\rm Pu}_{\rm chord},I} := [e_\iota]_{{\rm Pu}_\iota \in \mathcal{PU}_{{\rm chord},I}}$$

with the standard canonical basis vector $e_\iota \in \mathbb{R}^{n_{{\rm Pu}_I}}$, $n_{{\rm Pu}_I} := |\{{\rm Pu}_i \in \mathcal{C}_I\}|$. The pumps ${\rm Pu}_i \in \mathcal{P}_{{\rm cl},\iota}$ lying on the closed path associated with a chord ${\rm Pu}_\iota$ are selected by

$$\Pi_{\mathcal{P}_{{\rm cl},\iota}} := [e_i]_{{\rm Pu}_i \in \mathcal{P}_{{\rm cl},\iota}}, \tag{18}$$

for $e_i \in \mathbb{R}^{n_{{\rm Pu}_I}}$. The difference of the mass flows between the chord ${\rm Pu}_\iota$ and the pumps in $\mathcal{P}_{{\rm cl},\iota}$ is given by

$$[q_{{\rm Pu}_i} - q_{{\rm Pu}_\iota}]_{{\rm Pu}_i \in \mathcal{P}_{{\rm cl},\iota}} = \Pi^T_{\mathcal{P}_{{\rm cl},\iota}} (\Pi_{\mathcal{P}_{{\rm cl},\iota}} \Pi^T_{\mathcal{P}_{{\rm cl},\iota}} - (\mathbf{1}_I - e_\iota) e_\iota^T) q_{\rm Pu},$$

where $\mathbf{1}_I = [1, ..., 1]^T \in \mathbb{R}^{n_{{\rm Pu}_I}}$. The pumps lying on the spanning tree but not on any closed path are selected simply by

$$\Pi_{{\rm Pu}_{\rm tree} \setminus \mathcal{P}_{\rm cl},I} := [e_i]_{\mathcal{PU}_{{\rm tree},I} \setminus \{\cup_\iota \{\mathcal{P}_{{\rm cl},\iota} \cup \{{\rm Pu}_\iota\}\}\}}, \ e_i \in \mathbb{R}^{n_{{\rm Pu}_I}}. \tag{19}$$

From this, we define the variable transformation

$$\Pi_{q_{\mathrm{Pu}}} := \left[\Pi_{\mathrm{Pu}_{\mathrm{diff}}}\ \Pi_{\mathrm{Pu}_{\mathrm{chord}}}\right], \tag{20}$$

with $\Pi_{\mathrm{Pu}_{\mathrm{diff}}} := \mathrm{diag}(\Pi_{\mathrm{Pu}_{\mathrm{diff}},I})_{\mathcal{C}_I \in \mathcal{C}}$ given by

$$\Pi_{\mathrm{Pu}_{\mathrm{diff}},I} := \left[\Pi_{\mathrm{Pu}_{\mathrm{tree}} \setminus \mathcal{P}_{\mathrm{cl}},I},\ [\Pi^T_{\mathcal{P}_{\mathrm{cl},\iota}}(\Pi_{\mathcal{P}_{\mathrm{cl},\iota}}\Pi^T_{\mathcal{P}_{\mathrm{cl},\iota}} - (\mathbf{1}_I - e_\iota)e_\iota^T)]_{\mathrm{Pu}_\iota \in \mathcal{PU}_{\mathrm{chord},I}}\right],$$

and $\Pi_{\mathrm{Pu}_{\mathrm{chord}}} := \mathrm{diag}(\Pi_{\mathrm{Pu}_{\mathrm{chord}},I})_{\mathcal{C}_I \in \mathcal{C}}$. The associated variables are denoted by

$$q_i := \Pi_i^T q_{\mathrm{Pu}}, \quad i \in \{\mathrm{Pu}_{\mathrm{diff}}, \mathrm{Pu}_{\mathrm{chord}}\}.$$

The mass flow $q_{\mathrm{Pu}_{\mathrm{diff}}}$ comprises the mass flows in pumps lying on the spanning tree that are not part of a closed path as well as the mass flow difference of pumps lying on a closed path with respect to the associated chord pump. The mass flow $q_{\mathrm{Pu}_{\mathrm{chord}}}$ denotes the pump flow in the chord set.

For the equations, we proceed similarly as for the junction equations. We select all pumps lying on $\mathcal{PU}_{\mathrm{tree}}$ using the matrix $\Pi_{\mathrm{Pu}_{\mathrm{tree}}}$. For every chord $\mathrm{Pu}_\iota \in \mathcal{PU}_{\mathrm{chord}}$, we summarize this chord and the pumps on its closed path as super pump

$$\overline{\mathrm{Pu}}_\iota := \bigcup_{\mathrm{Pu}_i \in \mathcal{P}_{\mathrm{cl},\iota}} \mathrm{Pu}_i. \tag{21}$$

Algebraically, this identification is performed using the vector $\mathbf{1}_\iota$. Setting

$$\Pi_{\overline{\mathrm{Pu}}_\iota} := \mathrm{diag}(\mathbf{1}_\iota)_{\mathrm{Pu}_\iota \in \mathcal{PU}_{\mathrm{chord}}}$$

we construct our equation transformation as

$$\Pi_{F_{\mathrm{Pu}}} := \left[\Pi_{\mathrm{Pu}_{\mathrm{tree}}}\ \Pi_{\mathrm{Pu}_{\mathrm{clpath}}}\right], \tag{22}$$

with $\Pi_{\mathrm{Pu}_{\mathrm{tree}}} := \mathrm{diag}\left(\Pi_{\mathrm{Pu}_{\mathrm{tree}},I}\right)_{\mathcal{C}_I \in \mathcal{C}}$ and $\Pi_{\mathrm{Pu}_{\mathrm{clpath}}} := \mathrm{diag}(\Pi_{\mathrm{Pu}_{\mathrm{clpath}},I})_{\mathcal{C}_I \in \mathcal{C}}$ given by

$$\begin{aligned} \Pi_{\mathrm{Pu}_{\mathrm{tree}},I} &:= \left[\Pi_{\mathrm{Pu}_{\mathrm{tree}} \setminus \mathcal{P}_{\mathrm{cl}},I}\ \Pi_{\mathrm{Pu}_{\mathrm{tree}},I},\right], \\ \Pi_{\mathrm{Pu}_{\mathrm{clpath}},I} &:= [\mathbf{1}_{I,\iota}]_{\mathrm{Pu}_\iota \in \mathcal{PU}_{\mathrm{chord},I}}. \end{aligned}$$

The corresponding parts of the network function are given by

$$F_i := \Pi_i^T F_{\mathrm{Pu}}, \quad i \in \{\mathrm{Pu}_{\mathrm{tree}}, \mathrm{Pu}_{\mathrm{clpath}}\}. \tag{23}$$

The matrix $\Pi_{F_{\mathrm{Pu}}}$ filters out the regular and singular components of the incidence matrix $A_{\mathrm{Jc},\mathrm{Pu}}$.

Lemma 3 *[2] Consider $\Pi_{q_{Pu}}$ and $\Pi_{F_{Pu}}$ as defined in* (20) *and* (22)*.*

1. $\Pi^T_{q_{Pu}}\Pi_{F_{Pu}} = \Pi^T_{F_{Pu}}\Pi_{q_{Pu}} = I_{n_{Pu}}$.
2. $\mathrm{span}(\Pi_{Pu_{tree}}) = \mathrm{range}(A_{Jc,Pu})$ *and* $\mathrm{span}(\Pi_{Pu_{clpath}}) = \ker(A_{Jc,Pu})$.

Combining Lemma 1 and Lemma 3, we identify the regular components of the incidence matrix $A_{\mathrm{Jc},\mathrm{Pu}}$. Therefore, we set

$$A_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathrm{Pu}_{\mathrm{tree}}} := \Pi^T_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}} A_{\mathrm{Jc},\mathrm{Pu}} \Pi_{\mathrm{Pu}_{\mathrm{tree}}}, \tag{24}$$

and obtain the following result.

Corollary 1 *The matrix $A_{Jc_{\cancel{ref}},Pu_{tree}}$ as defined in* (24) *is non-singular with* $\mathrm{rank}(A_{Jc_{\cancel{ref}},Pu_{tree}}) = n_{Jc} - |\mathcal{C}_{\cancel{Re}}|$*. Furthermore, the equivalent relation* $\mathrm{rank}(A_{Jc_{\cancel{ref}},Pu_{tree}}) = n_{Pu} - |\mathcal{P}_{cl,reg}|$ *holds.*

Regarding the matrix D defined in (15), we set

$$\begin{aligned} D_{\text{tree}} &:= \Pi^T_{\text{Pu}_{\text{tree}}} D \Pi_{\text{Pu}_{\text{tree}}} \\ D_{\text{tree,clpath}} &:= \Pi^T_{\text{Pu}_{\text{tree}}} D \Pi_{\text{Pu}_{\text{clpath}}} \\ D_{\text{clpath}} &:= \Pi^T_{\text{Pu}_{\text{clpath}}} D \Pi_{\text{Pu}_{\text{clpath}}}. \end{aligned} \tag{25}$$

To specify the mass flow on the chord pumps, we observe the following.

Lemma 4 *Consider D_{clpath} as defined in (15). The matrix D_{clpath} is non-singular with $\operatorname{rank}(D_{clpath}) = |\mathcal{P}_{cl,reg}|$, if and only if Assumption 3 is satisfied.*

Proof By the construction of $\Pi_{\text{Pu}_{\text{clpath}}}$ and the diagonal structure of the matrix D, we have that $D_{\text{clpath}} = \operatorname{diag}(\sum_{\text{Pu}_i \in \mathcal{P}_{\text{cl},\iota}} D_{\text{Pu}_i,\text{Pu}_i})_{\iota \in \mathcal{PU}_{\text{chord}}}$, where $D_{\text{Pu}_i,\text{Pu}_i}$ refers to the entry of D associated with Pu_i. This matrix is non-singular if and only if $\sum_{\text{Pu}_i \in \mathcal{P}_{\text{cl},\iota}} D_{\text{Pu}_i,\text{Pu}_i} \neq 0$ for every $\iota \in \mathcal{PU}_{\text{chord}}$. However, this holds if and only if Assumption 3 is satisfied. □

Now, we turn to the pipes of the network. Graphically, the action of $\Pi_{F_{\text{Jc}}}$ corresponds to the *vertex identification* of the pump components $\mathcal{C}_{\text{Re}}$. For each $\mathcal{C}_I \in \mathcal{C}_{\text{Re}}$, this corresponds to melting the junctions $\text{Jc}_i \in \mathcal{C}_I$ into a single junction $\overline{\text{Jc}_I}$, i.e., we define the super junctions

$$\overline{\text{Jc}}_I := \bigcup_{\text{Jc}_i \in \mathcal{C}_I} \text{Jc}_i,$$

for $I = 1, ..., n_{\mathcal{C}_{\text{Re}}}$. For the FMU dependent and hidden constraint pump components, we summarize the junctions $\overline{\text{Jc}}_I$ arising from the vertex identification in the sets

$$\overline{\mathcal{JC}}_i := \left\{ \overline{\text{Jc}}_I | \; \mathcal{C}_I \in \mathcal{C}_{\text{Re},i} \right\}, \quad i \in \{\mathcal{B}_{\text{De}}, \text{HC}\}.$$

With these sets, we consider the graphs $\mathcal{G}_{\overline{\mathcal{JC}}_{\text{HC}},\text{Pi}} := \{\overline{\mathcal{JC}}_{\text{HC}}, \mathcal{PI}\}$ and $\mathcal{G}_{\overline{\mathcal{JC}}_{\mathcal{B}\text{De}},\text{Pi}} := \{\overline{\mathcal{JC}}_{\mathcal{B}_{\text{De}}}, \mathcal{PI}\}$, whose connection matrices are given by

$$A_{\star,\text{Pu}} := \Pi_\star^T A_{\text{Jc,Pu}}, \quad \star \in \{\mathcal{B}_{\text{De}}, \text{HC}\}. \tag{26}$$

For every connected component of the graph $\mathcal{G}_{\overline{\mathcal{JC}}_{\mathcal{B}_{\text{De}}},\text{Pi}} \cup \mathcal{G}_{\overline{\mathcal{JC}}_{\text{HC}},\text{Pi}}$, we once again choose a spanning tree, i.e., a largest subgraph without cycles, and summarize the associated pipes in $\mathcal{PI}_{\text{tree}}$. The associated chord set $\mathcal{PI}_{\text{chord}}$ contains the pipes closing cycles. The corresponding pipes are selected by the permutation

$$\Pi_{\text{Pi}} := [\Pi_{\text{Pi}_{\text{tree}}}, \Pi_{\text{Pi}_{\text{chord}}}], \tag{27}$$

where $\Pi_{\text{Pi}_{\text{tree}}} := [e_j]_{\text{Pi}_i \in \mathcal{PI}_{\text{tree}}}$ selects the pipes lying on the spanning tree and $\Pi_{\text{Pi}_{\text{chord}}} := [e_j]_{\text{Pi}_i \in \mathcal{PI}_{\text{chord}}}$ those on the chord set. The associated variables are given by

$$q_{\text{Pi}_i} := \Pi^T_{\text{Pi}_i} q_{\text{Pi}}, \quad i \in \{\text{tree}, \text{chord}\}.$$

The flow $q_{\text{Pi}_{\text{tree}}}$ denotes the pipe flows on the spanning tree of the super graph $\mathcal{G}_{\overline{\mathcal{JC}}_{\text{HC}},\text{Pi}} \cup \mathcal{G}_{\overline{\mathcal{JC}}_{\mathcal{B}_{\text{De}}},\text{Pi}}$, while $q_{\text{Pi}_{\text{chord}}}$ refers to the pipe flows on its chord set. The corresponding parts of the network function are given by

$$F_{\text{Pi}_i} := \Pi^T_{\text{Pi}_i} F_{\text{Pi}}, \quad i \in \{\text{tree}, \text{chord}\}. \tag{28}$$

To specify the flow $q_{\text{Pi}_{\text{chord}}}$ on the chord set as well as the pressure p_{HC} in the supernodes, we use $\Pi_{\text{Pi}_{\text{tree}}}$ and Π_{HC} given by (12), we set

$$A_{\text{HC},\text{Pi}_{\text{tree}}} := \Pi^T_{\text{HC}} A_{\text{Jc,Pi}} \Pi_{\text{Pi}_{\text{tree}}} \tag{29}$$

and make the following observation.

Lemma 5 *Consider Π_{Pi} and $A_{HC,Pi_{tree}}$ as in (27) and (29).*

1. *Then,* $\operatorname{corange}(A_{HC,Pi}) = \operatorname{span}(\Pi_{Pi_{tree}})$ *and $A_{HC,Pi_{tree}}$ is non-singular with* $\operatorname{rank}(A_{HC,Pi_{tree}}) = n_{HC}$.
2. *Let $f_{Pi,p_{Jc}}$ be the Jacobian of the pipe function f_{Pi} with respect to the junction pressure p_{Jc}. Then, $A_{HC,Pi_{tree}} f_{Pi,p_{Jc}}$ is non-singular with* $\operatorname{rank}(A_{HC,Pi_{tree}} f_{Pi,p_{Jc}}) = n_{HC}$.

Proof The proof follows from [2, Lemma 2.2] noting that $\overline{\text{Jc}}_{\text{HC}} \in \overline{\mathcal{JC}}_{\text{HC}}$ corresponds to the vertex identification of a liquid flow network without FMUs. □

6 Surrogate network functions

Using the substructures developed in Section 5, we define the surrogate network functions for the DAE model (2), (3) and (4). As the network function (5) is obtained by simply gluing together the single elements, the DAE (7) contains hidden constraints, which are equations that every solution has to satisfy but which are not contained explicitly in the network function (5). In order to make these hidden constraints visible for the solver and thus ensure a numerically stable solution, we consider the surrogate network function

$$\hat{F} = \left[F_{\mathcal{B}_{\mathrm{St}}}^T, F_{\mathrm{Pi}_{\mathrm{chord}}}^T, F_{\mathrm{Pu}}^T, F_{\mathrm{Jc}}^T, \hat{F}_{\mathrm{HC}}^T, F_{\mathcal{B}_{\mathrm{De}}}^T, F_{\mathcal{B}_{\mathrm{Re,Pi}}}^T, F_{\mathcal{B}_{\mathrm{Re,Pu}}}^T\right]^T, \tag{30}$$

with $F_{\mathcal{B}_{\mathrm{St}}}, F_{\mathrm{Pu}}, F_{\mathrm{Jc}}, F_{\mathcal{B}_{\mathrm{De}}}, F_{\mathcal{B}_{\mathrm{Re,Pi}}}, F_{\mathcal{B}_{\mathrm{Re,Pu}}}$ given by (6a), (6c) - (6g) and

$$F_{\mathrm{Pi}_{\mathrm{chord}}} := \Pi_{\mathrm{Pi}_{\mathrm{chord}}}^T \dot{q}_{\mathrm{Pi}} - \Pi_{\mathrm{Pi}_{\mathrm{chord}}}^T f_{\mathrm{Pi}}(q_{\mathrm{Pi}}, p_{\mathrm{Jc}}, \bar{p}_{\mathrm{Re}}, y_{\mathrm{Re,Pi}}) \tag{31a}$$

$$\hat{F}_{\mathrm{HC}} := \dot{g}_{\overline{\mathrm{Jc}}_{\mathrm{HC}}} + A_{\mathrm{HC,Pi}} f_{\mathrm{Pi}}(q_{\mathrm{Pi}}, p_{\mathrm{Jc}}, y_{\mathrm{Re,Pi}}, \bar{p}_{\mathrm{Re}}) + A_{\mathrm{HC,De}} \dot{\bar{q}}_{\mathrm{De}}. \tag{31b}$$

The equation $\hat{F}_{\mathrm{HC}}(X) = 0$ are called *hidden constraints*. The surrogate network function $\hat{F}$ is constructed explicitly in the proof of Theorem 1 and the surrogate model is given by

$$\hat{F}(X) = 0. \tag{32}$$

The surrogate model (32) involves the same variables as the original system, i.e., no variable transformation is necessary. However, the number of differential and algebraic equations in (32) differs from those of the DAE (7) as they are given by

$$\hat{d} := n_{\mathrm{St}} + n_{\mathrm{Pi}} - n_{\mathrm{HC}} \tag{33a}$$

$$\hat{a} := n_{\mathrm{De}_c} + n_{\mathrm{Re}_c} + n_{\mathrm{Jc}} + n_{\mathrm{Pu}} + n_{\mathrm{HC}} \tag{33b}$$

cp. (8). Again, we summarize the differential and algebraic equations in (32) by

$$\hat{F}_{\hat{d}} := [F_{\mathrm{Pi}_{\mathrm{chord}}}^T, F_{\mathcal{B}_{\mathrm{St}}}^T]^T,$$
$$\hat{F}_{\hat{a}} := [F_{\mathrm{Jc}}^T, F_{\mathrm{Pu}}^T, \hat{F}_{\mathrm{HC}}^T, F_{\mathcal{B}_{\mathrm{De}}}^T, F_{\mathcal{B}_{\mathrm{Re,Pi}}}^T, F_{\mathcal{B}_{\mathrm{Re,Pu}}}^T]^T$$

and the differential and algebraic variables by

$$\hat{X}_{\hat{d}} := [q_{\mathrm{Pi}_{\mathrm{chord}}}^T, x^T]^T,$$
$$\hat{X}_{\hat{a}} := [q_{\mathrm{Pi}_{\mathrm{tree}}}^T, p_{\mathrm{Jc}}^T, y_{\mathrm{De}}^T, q_{\mathrm{Pu}}^T, y_{\mathrm{Re,Pi}}^T, y_{\mathrm{Re,Pu}}^T]^T.$$

Given the surrogate network function $\hat{F}$, we define the set of consistent initial values for the DAE (7) as

$$\mathcal{C}_{IV} := \{(t_0, X_0) \in \mathcal{I} \times \mathbb{R}^n \mid \hat{F}_{\hat{a}}(t_0, X_0) = 0\},$$

i.e., a state X_0 is consistent for the DAE (7), if X_0 solves the algebraic equations of the surrogate model.

Regarding the smoothness of the network function F, we make the following observation.

Lemma 6 *Consider the network function F as defined in* (5). *Let $f_{Pu} \in C^1(\Omega_{n_{Pu}}, \mathbb{R}^{n_{Pu}})$, $\bar{q}_{De} \in C^1(\mathcal{I}_{De}, \mathbb{R}^{n_{De_e}})$, $\bar{p}_{Re} \in C^1(\mathcal{I}_{Re}, \mathbb{R}^{n_{Re_e}})$ and $f_{St} \in C(\mathcal{I}_{St} \times \mathbb{R}^{n_{St}} \times \Omega_{\star_c}, \mathbb{R}^{n_{St}})$, $g_\star \in C(\mathcal{I}_\star \times \mathbb{R}^{n_{St,\star}} \times \Omega_{\star_c}, \mathbb{R}^{n_{\star_c}})$, $\star \in \{De, (Re, Pi), (Re, Pu)\}$ with $g_{\mathcal{B}_{De}} \in C^1(\mathcal{I}_{De} \times \mathbb{R}^{n_{St,De}} \times \Omega_{De_c}, \mathbb{R}^{n_{De_c}})$. Then, $F \in C(\mathcal{I} \times \mathbb{R}^n \times \mathbb{R}^n, \mathbb{R}^n)$ with $F_\star \in C^1(\mathcal{I}_\star \times \mathbb{R}^{n_{\star_e}}, \mathbb{R}^{n_{\star_e}})$, $\star \in \{De, Re\}$, and $F_{\mathcal{B}_{De}} \in C^1(\mathcal{I}_{De} \times \mathbb{R}^{n_{St,De}} \times \Omega_{De_c}, \mathbb{R}^{n_{De_c}})$, in particular.*

Proof The pipe function f_{Pi} as considered in (2a) satisfies $f_{\mathrm{Pi}} \in C(\mathbb{R}^{n_{\mathrm{Pi}}} \times \mathbb{R}^{n_{\mathrm{Jc}}} \times \mathbb{R}^{n_{\mathrm{Re}}}, \mathbb{R}^{n_{\mathrm{Pi}}})$. For a given mass flow q_{Pi}, we even have $f_{\mathrm{Pi}}(q_{\mathrm{Pi}}, \cdot, \cdot) \in C^1(\mathbb{R}^{n_{\mathrm{Jc}}} \times \mathbb{R}^{n_{\mathrm{Re}}}, \mathbb{R}^{n_{\mathrm{Pi}}})$. Hence, $F_{\mathrm{Pi}} \in C(\mathbb{R}^n, \mathbb{R}^{n_{\mathrm{Pi}}})$ and $F_{\mathrm{Pi}}(q_{\mathrm{Pi}}, \cdot, \cdot) \in C^1(\mathbb{R}^{n_{\mathrm{Jc}}} \times \mathbb{R}^{n_{\mathrm{Re}}}, \mathbb{R}^{n_{\mathrm{Pi}}})$ for given mass flow q_{Pi}. For the pump function, we note that $F_{\mathrm{Pu}} \in C^1(\mathbb{R}^n, \mathbb{R}^{n_{\mathrm{Pu}}})$ if $f_{\mathrm{Pu}} \in C^1(\mathbb{R}^{n_{\mathrm{Pu}}}, \mathbb{R}^{n_{\mathrm{Pu}}})$. As the mass balance is linear, we get that $F_{\mathrm{Jc}} \in C^1(\mathbb{R}^n, \mathbb{R}^{n_{\mathrm{Jc}}})$. For the demand and reservoir functions, we have that $F_\star \in C^1(\mathcal{I}_\star \times \mathbb{R}^{n_{\star_e}}, \mathbb{R}^{n_{\star_e}})$, $\star \in \{\mathrm{De}, \mathrm{Re}\}$ if $\bar{q}_{\mathrm{De}} \in C^1(\mathcal{I}, \mathbb{R}^{n_{\mathrm{De}_e}})$ and $\bar{q}_{\mathrm{Re}} \in C^1(\mathcal{I}, \mathbb{R}^{n_{\mathrm{Re}_e}})$.

For the FMUs, we have that $F_{\mathcal{B}_{\mathrm{St}}} \in C(\mathbb{R}^n, \mathbb{R}^{n_{\mathrm{St}}})$ if the state functions are $f_{\mathrm{St}} \in C(\mathbb{R}^n, \mathbb{R}^{n_{\mathrm{St}}})$. Furthermore, $F_{\mathcal{B}_{\mathrm{De}}} \in C(\mathcal{I} \times \mathbb{R}^{n_{\mathrm{St}}} \times \mathbb{R}^{n_{\mathrm{De}_c}}, \mathbb{R}^{n_{\mathrm{De}_c}})$ and $F_{\mathcal{B}_{\mathrm{Re},i}} \in C(\mathcal{I} \times \mathbb{R}^{n_{\mathrm{St}}} \times \mathbb{R}^{n_{i_c}}, \mathbb{R}^{n_{i_c}})$ for $i \in \{\mathrm{Pi}, \mathrm{Pu}\}$ if $g_{\mathrm{De}} \in C(\mathbb{R}^n, \mathbb{R}^{n_{\mathrm{De}_c}})$, $g_{\mathrm{Re,Pi}} \in C(\mathbb{R}^n, \mathbb{R}^{n_{\mathrm{Re,Pi}_c}})$ and $g_{\mathrm{Re,Pu}} \in C(\mathbb{R}^n, \mathbb{R}^{n_{\mathrm{Re,Pu}_c}})$. For the demand FMUs, in particular, we have that $F_{\mathcal{B}_{\mathrm{De}}} \in C^1(\mathcal{I} \times \mathbb{R}^{n_{\mathrm{St}}} \times \mathbb{R}^{n_{\mathrm{De}_c}}, \mathbb{R}^{n_{\mathrm{De}_c}})$ if $g_{\mathcal{B}_{\mathrm{De}}} \in C^1(\mathbb{R}^n, \mathbb{R}^{n_{\mathrm{De}_c}})$. □

7 Solvability results

Having introduced the relevant structures of the network, we use this information to characterize the solvability of the network model (7). Therefore, we need the rank of certain partial derivatives arising in the DAE analysis. In particular the time derivative $\dot{F}$ of the network function F is needed, which is given by

$$\dot{F}_{\mathcal{B}_{\mathrm{St}}} = \ddot{x} - F_{\mathrm{St},t} - F_{\mathrm{St},x}\dot{x} - F_{\mathrm{St},p_{\mathrm{Jc}_c}}\dot{p}_{\mathrm{Jc}_c} - F_{\mathrm{St},q_{\mathrm{Pi}_c}}\dot{q}_{\mathrm{Pi}_c} - F_{\mathrm{St},q_{\mathrm{Pu}_c}}\dot{q}_{\mathrm{Pu}_c} \tag{34a}$$

$$\dot{F}_{\mathrm{Pi}} = \ddot{q}_{\mathrm{Pi}} - f_{\mathrm{Pi},q_{\mathrm{Pi}}}\dot{q}_{\mathrm{Pi}} - f_{\mathrm{Pi},p_{\mathrm{Jc}}}\dot{p}_{\mathrm{Jc}} - f_{\mathrm{Pi}_c,y_{\mathrm{Re}}}\dot{y}_{\mathrm{Re}} - f_{\mathrm{Pi},\bar{p}_{\mathrm{Re}}}\dot{\bar{p}}_{\mathrm{Re}} \tag{34b}$$

$$\dot{F}_{\mathrm{Pu}} = A^T_{\mathrm{Jc,Pu}}\dot{p}_{\mathrm{Jc}} + \dot{y}_{\mathrm{Re,Pu}} + A^T_{\mathrm{Re}_e,\mathrm{Pu}}\dot{\bar{p}}_{\mathrm{Re}_e} - f_{\mathrm{Pu},q_{\mathrm{Pu}}}\dot{q}_{\mathrm{Pu}} \tag{34c}$$

$$\dot{F}_{\mathrm{Jc}} = A_{\mathrm{Jc,Pi}}\dot{q}_{\mathrm{Pi}} + A_{\mathrm{Jc,Pu}}\dot{q}_{\mathrm{Pu}} + \dot{y}_{\mathrm{De}} + A_{\mathrm{Jc,De}}\dot{\bar{q}}_{\mathrm{De}} \tag{34d}$$

$$\dot{F}_{\mathcal{B}_{\mathrm{De}}} = \dot{y}_{\mathrm{De}} - g_{\mathrm{De},t} - g_{\mathrm{De},x}\dot{x} - g_{\mathrm{De},p_{\mathrm{Jc}_c}}\dot{p}_{\mathrm{Jc}_c} \tag{34e}$$

$$\dot{F}_{\mathcal{B}_{\mathrm{Re,Pi}}} = \dot{y}_{\mathrm{Re,Pi}} - g_{\mathrm{Re,Pi},t} - g_{\mathrm{Re,Pi},x}\dot{x} - g_{\mathrm{Re,Pi},q_{\mathrm{Pi}_c}}\dot{q}_{\mathrm{Pi}_c} \tag{34f}$$

$$\dot{F}_{\mathcal{B}_{\mathrm{Re,Pu}}} = \dot{y}_{\mathrm{Re,Pu}} - g_{\mathrm{Re,Pu},t} - g_{\mathrm{Re,Pu},x}\dot{x} - g_{\mathrm{Re,Pu},q_{\mathrm{Pu}_c}}\dot{q}_{\mathrm{Pu}_c}. \tag{34g}$$

Therefore, the rank of certain partial derivatives arising in the DAE analysis has to be determined. First, we compute the rank and a basis of the cokernel of the partial derivatives.

$$\dot{F}_{a,\dot{X}_a} = \begin{bmatrix} I_{n_{\mathrm{Pi}_c}} & 0 & 0 & 0 & 0 \\ 0 & I_{n_{\mathrm{Pu}_c}} & 0 & [0, -g_{\mathrm{Re,Pu},q_{\mathrm{Pu}_c}}]^T & 0 \\ 0 & 0 & I_{n_{\mathrm{Jc}_c}} & 0 & [0, -g_{\mathrm{De},p_{\mathrm{Jc}_c}}]^T \\ 0 & 0 & [0, I_{n_{\mathrm{Jc}_c}}]^T & A_{\mathrm{Jc,Pu}} & 0 \\ 0 & [0, I_{n_{\mathrm{Pu}_c}}]^T & 0 & -f_{\mathrm{Pu},q_{\mathrm{Pu}}} & A^T_{\mathrm{Jc,Pu}} \end{bmatrix}. \tag{35}$$

Indeed, this is the partial derivative of the algebraic equations in the DAE (7) with respect to the algebraic variables.

Lemma 7 *Consider the matrix* $\dot{F}_{a,\dot{X}_a}$ *given in* (35). *Let Assumption 2 and Assumption 3 be satisfied. Then,* $\mathrm{rank}(\dot{F}_{a,\dot{X}_a}) = a - n_{HC}$. *Using* $\Pi_{HC,c}$ *and* Π_{HC} *given by* (12), *a matrix* $Z_{22} \in \mathbb{R}^{a \times n_{C_{HC}}}$ *fulfilling* $\mathrm{span}(Z_{22}) = \mathrm{coker}(\dot{F}_{a,\dot{X}_a})$ *is given by*

$$Z_{22}^T = \left[0,\, 0,\, -\Pi_{HC,c}^T,\, \Pi_{HC}^T,\, 0\right]. \tag{36}$$

Proof To determine $\operatorname{rank}(\dot{F}_{a,\dot{X}_a})$, we use Gaussian block elimination as well as the matrices $\mathit{\Pi}_{F_{\mathrm{Jc}}}$ and $\mathit{\Pi}_{F_{\mathrm{Pu}}}$ defined in (12) and (22) to filter out the non-singular components. Setting

$$L = \begin{bmatrix} I_{n_{\mathrm{Re}_c,\mathrm{Pi}}} & 0 & 0 & 0 & 0 \\ 0 & I_{n_{\mathrm{Re}_c,\mathrm{Pu}}} & 0 & 0 & 0 \\ 0 & 0 & I_{n_{\mathrm{De}_c}} & 0 & 0 \\ 0 & -\mathit{\Pi}^T_{\overline{\mathrm{Pu}},c} & -D^T_{\mathrm{tree,clpath}} A^{-1}_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathrm{Pu}_{\mathrm{tree}}} \mathit{\Pi}^T_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},c} & D^T_{\mathrm{tree,clpath}} A^{-1}_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathrm{Pu}_{\mathrm{tree}}} \mathit{\Pi}^T_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}} & \mathit{\Pi}^T_{\mathrm{Pu}_{\mathrm{clpath}}} \\ 0 & 0 & -\mathit{\Pi}^T_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},c} & \mathit{\Pi}^T_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}} & 0 \\ 0 & 0 & -\mathit{\Pi}^T_{\mathcal{B}_{\mathrm{De}},c} & \mathit{\Pi}^T_{\mathcal{B}_{\mathrm{De}}} & 0 \\ 0 & -\mathit{\Pi}^T_{\mathrm{Pu}_{\mathrm{tree}},c} & -D_{\mathrm{tree}} A^{-1}_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathrm{Pu}_{\mathrm{tree}}} \mathit{\Pi}^T_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},c} & D_{\mathrm{tree}} A^{-1}_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathrm{Pu}_{\mathrm{tree}}} \mathit{\Pi}^T_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}} & \mathit{\Pi}^T_{\mathrm{Pu}_{\mathrm{tree}}} \\ 0 & 0 & -\mathit{\Pi}^T_{\mathrm{HC},c} & \mathit{\Pi}^T_{\mathrm{HC}} & 0 \end{bmatrix},$$

where we have used the definitions in (25), and

$$R = \begin{bmatrix} I_{n_{\mathrm{De}_c}+n_{\mathrm{Re}_c}} & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathit{\Pi}_{\mathrm{Pu}_{\mathrm{clpath}}} & \mathit{\Pi}_{\mathrm{Pu}_{\mathrm{tree}}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathit{\Pi}_{\mathcal{B}_{\mathrm{De}}} & \mathit{\Pi}_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}} & \mathit{\Pi}_{\mathrm{HC}} \end{bmatrix},$$

we find that

$$L\dot{F}_{a,\dot{X}_a} R = \begin{bmatrix} I_{n_{\mathrm{De}_c}+n_{\mathrm{Re}_c}} & * & * \\ 0 & B_{22} & 0 \\ 0 & 0 & 0 \end{bmatrix}, \tag{37}$$

with

$$B_{22} := \begin{bmatrix} -D_{\mathrm{clpath}} & 0 & -D^T_{\mathrm{tree,clpath}} A^{-1}_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathrm{Pu}_{\mathrm{tree}}} G_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathcal{B}_{\mathrm{De}}} & -D^T_{\mathrm{tree,clpath}} A^{-1}_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathrm{Pu}_{\mathrm{tree}}} G_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}} \\ 0 & A_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathrm{Pu}_{\mathrm{tree}}} & -G_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathcal{B}_{\mathrm{De}}} & -G_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}} \\ 0 & 0 & -G_{\mathcal{B}_{\mathrm{De}}} & -G^T_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathcal{B}_{\mathrm{De}}} \\ 0 & 0 & 0 & A^T_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathrm{Pu}_{\mathrm{tree}}} - D_{\mathcal{S}} A^{-1}_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathrm{Pu}_{\mathrm{tree}}} G_{\mathcal{S}} \end{bmatrix}.$$

The Schur complements $G_{\mathcal{S}}$ and $D_{\mathcal{S}}$ are given by

$$G_{\mathcal{S}} := G_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}} - G_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathcal{B}_{\mathrm{De}}} G^{-1}_{\mathcal{B}_{\mathrm{De}}} G^T_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathcal{B}_{\mathrm{De}}},$$
$$D_{\mathcal{S}} := D_{\mathrm{tree}} - D_{\mathrm{tree,clpath}} D^{-1}_{\mathrm{clpath}} D^T_{\mathrm{tree,clpath}}.$$

Given Assumption 2, we have $G_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}} = 0$ and $G_{\mathrm{Jc}_{\cancel{\mathrm{ref}}},\mathcal{B}_{\mathrm{De}}} = 0$, cp. Lemma 2, which implies that $G_{\mathcal{S}} = 0$. By Lemma 2 and Lemma 4 and the construction of $\mathit{\Pi}_{\mathrm{Jc}_{\cancel{\mathrm{ref}}}}, \mathit{\Pi}_{\mathrm{Pu}_{\mathrm{tree}}}$, the diagonal entries of B_{22} are non-singular, implying that

$$\operatorname{rank}(B_{22}) = 2n_{\mathrm{Jc}} - 2n_{\mathcal{C}_{\cancel{\mathrm{Re}}}} + n_{\mathcal{B}_{\mathrm{De}}} + |\mathcal{P}_{\mathrm{cl,reg}}|$$

and $\operatorname{coker}(B_{22}) = \{0\}$. Noting that $n_{\mathrm{Pu}} = n_{\mathcal{C}_{\mathrm{Re}}} + |\mathcal{P}_{\mathrm{cl,reg}}|$, cp. Corollary 1, and $n_{\mathrm{Jc}} - n_{\mathcal{C}_{\cancel{\mathrm{Re}}}} = n_{\mathcal{C}_{\mathrm{Re}}}$, we find that $\operatorname{rank}(B_{22}) = n_{\mathrm{Jc}} + n_{\mathrm{Pu}} - n_{\mathrm{HC}}$. Using the decomposition (37), we obtain $\operatorname{rank}(\dot{F}_{a,X_a})$ and Z_{22} as proposed above. □

With the matrix Z_{22} and the Jacobian $\dot{F}_{a,\dot{X}_d}$ given by

$$\dot{F}_{a,\dot{X}_d} = \begin{bmatrix} -g_{\mathrm{Re,Pi},x} & [0, -g_{\mathrm{Re,Pi},q_{\mathrm{Pi}_c}}] \\ -g_{\mathrm{Re,Pu},x} & 0 \\ -g_{\mathrm{De},x} & 0 \\ 0 & A_{\mathrm{Jc,Pi}} \\ 0 & 0 \end{bmatrix}, \tag{38}$$

we consider the matrix

$$\bar{N} := \begin{bmatrix} F_{a,X} \\ Z_{22}^T(\dot{F}_{a,X} - \dot{F}_{a,\dot{X}_d} F_{d,X}) \end{bmatrix}. \tag{39}$$

Straightforward computations yield

$$\bar{N} = \begin{bmatrix} I_{n_{\mathrm{Jc_c}}} & 0 & 0 & 0 & 0 & [0, -g_{\mathrm{De},p_{\mathrm{Jc_c}}}] & -g_{\mathrm{De},x} \\ 0 & I_{n_{\mathrm{Pi_c}}} & 0 & [0, -g_{\mathrm{Re,Pi},q_{\mathrm{Pi_c}}}] & 0 & 0 & -g_{\mathrm{Re,Pi},x} \\ 0 & 0 & I_{n_{\mathrm{Pu_c}}} & 0 & [0, -g_{\mathrm{Re,Pu},q_{\mathrm{Pu_c}}}] & 0 & -g_{\mathrm{Re,Pu},x} \\ [0, I_{n_{\mathrm{Jc_c}}}]^T & 0 & 0 & A_{\mathrm{Jc,Pi}} & A_{\mathrm{Jc,Pu}} & 0 & 0 \\ 0 & 0 & [0, I_{n_{\mathrm{Pu_c}}}]^T & 0 & -f_{\mathrm{Pu},q_{\mathrm{Pu}}} & A_{\mathrm{Jc,Pu}}^T & 0 \\ 0 & A_{\mathrm{HC,Pi}} f_{\mathrm{Pi_c},y_{\mathrm{Re,Pi}}} & 0 & b_{\mathrm{HC},q_{\mathrm{Pi}}} & g_{\mathrm{HC},x}[0, F_{\mathrm{St},q_{\mathrm{Pu_c}}}] & A_{\mathrm{HC,Pi}} f_{\mathrm{Pi},p_{\mathrm{Jc}}} & b_{\mathrm{HC},x} \end{bmatrix}$$

where the last block row corresponds to $Z_{22}^T \dot{F}_{a,X} - Z_{22}^T \dot{F}_{a,\dot{X}_d} F_{d,X}$ and

$$\begin{aligned} b_{\mathrm{HC},q_{\mathrm{Pi}}} &:= g_{\mathrm{HC},x}[0, F_{\mathrm{St},q_{\mathrm{Pi_c}}}] + A_{\mathrm{HC,Pi}} f_{\mathrm{Pi},q_{\mathrm{Pi}}}, \\ b_{\mathrm{HC},x} &:= \dot{g}_{\mathrm{HC},x} + g_{\mathrm{HC},x} F_{\mathrm{St},x}. \end{aligned}$$

Lemma 8 *Consider the matrix $\bar{N}$ as given in (39). Let Assumption 2 and Assumption 3 be satisfied. Then,* $\mathrm{rank}(\bar{N}) = \hat{a}$ *, where $\hat{a}$ is given as in (33). Furthermore, there exists a basis $T_2 \in \mathbb{R}^{n \times \hat{d}}$ with* $\mathrm{span}(T_2) = \ker(\bar{N})$ *such that*

$$[I_{n_{Pi}+n_{St}}, 0] T_2 = \begin{bmatrix} -\Pi_{Pi_{tree}} A_{HC,Pi_{tree}}^{-1} g_{HC,x} & \Pi_{Pi_{chord}} - \Pi_{Pi_{tree}} A_{HC,Pi_{chord}} \\ I_{n_{St}} & 0 \end{bmatrix}.$$

Proof To determine $\mathrm{rank}(\bar{N})$, we again use Gaussian block elimination as well as the matrices $\Pi_{F_{\mathrm{Jc}}}$, $\Pi_{F_{\mathrm{Pu}}}$, and Π_{Pi} defined in (12), (22), and (27) to filter out the non-singular components. Setting

$$L_{22} = \begin{bmatrix} \Pi_{\mathrm{HC}}^T & 0 & 0 \\ \Pi_{\mathcal{B}_{\mathrm{De}}}^T & 0 & 0 \\ \Pi_{\mathrm{Jc_{ref}}}^T & 0 & 0 \\ 0 & \Pi_{\mathrm{Pu_{clpath}}}^T & 0 \\ 0 & \Pi_{\mathrm{Pu_{tree}}}^T & 0 \\ 0 & 0 & I_{n_{\mathrm{HC}}} \end{bmatrix} \tag{40}$$

and $\bar{R} = [\bar{R}_{ij}]_{i=1,2,j=2,3}$ with

$$\bar{R}_{12} = \begin{bmatrix} 0 & [0, g_{\mathrm{De},p_{\mathcal{B}_{\mathrm{De}},c}}] & 0 & 0 & [0, g_{\mathrm{De},p_{\mathrm{diff},c}}] & [0, g_{\mathrm{De},p_{\mathrm{HC},c}}] \\ [0, g_{\mathrm{Re,Pi},q_{\mathrm{Pi_{tree}},c}}] & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & [0, g_{\mathrm{Re,Pu},q_{\mathrm{Pu_{diff}},c}}] & [0, g_{\mathrm{Re,Pu},q_{\mathrm{Pu_{chord}},c}}] & 0 & 0 \end{bmatrix},$$

$$\bar{R}_{13} = \begin{bmatrix} 0 & g_{\mathrm{De},x} \\ [0, g_{\mathrm{Re,Pi},q_{\mathrm{Pi_{chord}},c}}] & g_{\mathrm{Re,Pi},x} \\ 0 & g_{\mathrm{Re,Pu},x} \end{bmatrix}, \quad \bar{R}_{23} = \begin{bmatrix} 0 & \Pi_{\mathrm{Pi_{chord}}} \\ 0 & 0 \\ 0 & 0 \\ I_{n_{\mathrm{St}}} & 0 \end{bmatrix},$$

$$\bar{R}_{22} = \begin{bmatrix} \Pi_{\mathrm{Pi_{tree}}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \Pi_{\mathrm{Pu_{tree}}} & \Pi_{\mathrm{Pu_{clpath}}} & 0 & 0 \\ 0 & \Pi_{\mathcal{B}_{\mathrm{De}}} & 0 & 0 & \Pi_{\mathrm{Jc_{ref}}} & \Pi_{\mathrm{HC}} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \tag{41}$$

we obtain the decomposition

$$\begin{bmatrix} I_{n_{\mathrm{De_c}}+n_{\mathrm{Re_c}}} & 0 \\ 0 & L_{22} \end{bmatrix} \bar{N} \begin{bmatrix} I_{n_{\mathrm{De_c}}+n_{\mathrm{Re_c}}} & \bar{R}_{12} & \bar{R}_{13} \\ 0 & \bar{R}_{22} & \bar{R}_{23} \end{bmatrix} = \begin{bmatrix} I_{n_{\mathrm{De_c}}+n_{\mathrm{Re_c}}} & 0 & 0 \\ * & \bar{N}_{22} & \bar{N}_{23} \end{bmatrix}, \tag{42}$$

with

$$\bar{N}_{22} = \begin{bmatrix} A_{\mathrm{HC},\mathrm{Pi}_{\mathrm{tree}}} & 0 & 0 & 0 & 0 & 0 \\ A_{\mathcal{B}_{\mathrm{De}},\mathrm{Pi}_{\mathrm{tree}}} & G_{\mathcal{B}_{\mathrm{De}}} & 0 & 0 & G^T_{\mathrm{Jc}_{\mathrm{ref}},\mathcal{B}_{\mathrm{De}}} & 0 \\ A_{\mathrm{Jc}_{\mathrm{ref}},\mathrm{Pi}_{\mathrm{tree}}} & G_{\mathrm{Jc}_{\mathrm{ref}},\mathcal{B}_{\mathrm{De}}} & A_{\mathrm{Jc}_{\mathrm{ref}},\mathrm{Pu}_{\mathrm{tree}}} & 0 & G_{\mathrm{Jc}_{\mathrm{ref}}} & 0 \\ 0 & 0 & D^T_{\mathrm{tree},\mathrm{clpath}} & D_{\mathrm{clpath}} & 0 & 0 \\ 0 & 0 & D_{\mathrm{tree}} & D_{\mathrm{tree},\mathrm{clpath}} & A^T_{\mathrm{Jc}_{\mathrm{ref}},\mathrm{Pu}_{\mathrm{tree}}} & 0 \\ b_{\mathrm{HC},q_{\mathrm{Pi}_{\mathrm{tree}}}} & b_{\mathrm{HC},p_{\mathcal{B}_{\mathrm{De}}}} & b_{\mathrm{HC},q_{\mathrm{Pu}_{\mathrm{diff}}}} & b_{\mathrm{HC},q_{\mathrm{Pu}_{\mathrm{chord}}}} & b_{\mathrm{HC},p_{\mathrm{diff}}} & b_{\mathrm{HC},p_{\mathrm{HC}}} \end{bmatrix},$$

$$\bar{N}_{23} = \begin{bmatrix} g_{\mathrm{HC},x} & A_{\mathrm{HC},\mathrm{Pi}_{\mathrm{chord}}} \\ g_{\mathrm{Jc}_{\mathrm{ref}},x} & A_{\mathrm{Jc}_{\mathrm{ref}},\mathrm{Pi}_{\mathrm{chord}}} \\ g_{\mathrm{Pu}_{\mathrm{tree}},x} & 0 \\ g_{\mathrm{Pu}_{\mathrm{clpath}},x} & 0 \\ g_{\mathcal{B}_{\mathrm{De}},x} & A_{\mathcal{B}_{\mathrm{De}},\mathrm{Pi}_{\mathrm{chord}}} \\ b_{\mathrm{HC},x} & b_{\mathrm{HC},q_{\mathrm{Pi}_{\mathrm{chord}}}} \end{bmatrix}.$$

Here, we have already used Assumption 2, implying that $G_{\mathrm{Jc}_{\mathrm{ref}}} = 0$ and $G_{\mathrm{Jc}_{\mathrm{ref}},\mathcal{B}_{\mathrm{De}}} = 0$. The diagonal elements of $\bar{N}_{22}$ are non-singular by Lemma 2 and Lemma 4. Hence, we get

$$\mathrm{rank}(\bar{N}_{22}) = n_{\mathrm{Jc}} + n_{\mathrm{Pu}} + n_{\mathrm{HC}}.$$

Using the decomposition (42), we obtain the proposed rank of $\hat{N}$. Regarding the decomposition (42), a basis T_2 of $\ker(\bar{N})$ is given by

$$T_2 = \begin{bmatrix} \bar{R}_{13} - \bar{R}_{12}\bar{N}_{22}^{-1}\bar{N}_{23} \\ \bar{R}_{23} - \bar{R}_{22}\bar{N}_{22}^{-1}\bar{N}_{23} \end{bmatrix}.$$

Computing the rows of T_2 associated with the differential variables q_{Pi}, x, we obtain T_2 as proposed. Decomposing the block row associated with the pipes using $\Pi_{\mathrm{Pi}_{\mathrm{tree}}}$, $\Pi_{\mathrm{Pi}_{\mathrm{chord}}}$ and noting that $\Pi^T_{\mathrm{Pi}_i}\Pi_{\mathrm{Pi}_j} = \delta_{ij} I_{n_{\mathrm{Pi}_i}}$, $i, j \in \{\mathrm{tree}, \mathrm{chord}\}$, as $[\Pi_{\mathrm{Pi}_{\mathrm{tree}}}, \Pi_{\mathrm{Pi}_{\mathrm{chord}}}]$ is a permutation, we find that there exists a permutation P, such that

$$P^T T_2 = \begin{bmatrix} * & * \\ * & * \\ * & * \\ -A^{-1}_{\mathrm{HC},\mathrm{Pi}_{\mathrm{tree}}} g_{\mathrm{HC},x} & -\Pi_{\mathrm{Pi}_{\mathrm{tree}}} A_{\mathrm{HC},\mathrm{Pi}_{\mathrm{chord}}} \\ 0 & I_{n_{\mathrm{Pi}_{\mathrm{chord}}}} \\ * & * \\ * & * \\ I_{n_{\mathrm{St}}} & 0 \end{bmatrix},$$

i.e., $\mathrm{rank}(T_2) = d$. □

For the surrogate model (32), we consider the Jacobian of the algebraic equations $\hat{F}_{\hat{a}}$ in (32) with respect to the algebraic variables $\hat{X}_a$, i.e.,

$$\hat{F}_{\hat{a},\hat{X}_a} = \begin{bmatrix} I_{n_{\mathrm{Jc}_c}} & 0 & 0 & 0 & 0 & [0, -g_{\mathrm{De},p_{\mathrm{Jc}_c}}] \\ 0 & I_{n_{\mathrm{Pi}_c}} & 0 & [0, -g_{\mathrm{Re},\mathrm{Pi},q_{\mathrm{Pi}_{\mathrm{tree}},c}}] & 0 & 0 \\ 0 & 0 & I_{n_{\mathrm{Pu}_c}} & 0 & [0, -g_{\mathrm{Re},\mathrm{Pu},q_{\mathrm{Pu}_c}}] & 0 \\ [0, I_{n_{\mathrm{Jc}_c}}]^T & 0 & 0 & A_{\mathrm{Jc},\mathrm{Pi}_{\mathrm{tree}}} & A_{\mathrm{Jc},\mathrm{Pu}} & 0 \\ 0 & 0 & [0, I_{n_{\mathrm{Pu}_c}}]^T & 0 & -f_{\mathrm{Pu},q_{\mathrm{Pu}}} & A^T_{\mathrm{Jc},\mathrm{Pu}} \\ 0 & A_{\mathrm{HC},\mathrm{Pi}} f_{\mathrm{Pi},y_{\mathrm{Re},\mathrm{Pi}}} & 0 & A_{\mathrm{HC},\mathrm{Pi}} f_{\mathrm{Pi},q_{\mathrm{Pi}_{\mathrm{tree}}}} & 0 & A_{\mathrm{HC},\mathrm{Pi}} f_{\mathrm{Pi},p_{\mathrm{Jc}}} \end{bmatrix}. \quad (43)$$

Lemma 9 *Consider the Jacobian* (43)*. Let Assumption 2 and 3 be satisfied. Then,* $\hat{F}_{\hat{a},\hat{X}_a}$ *is non-singular.*

Proof Considering the transformations L_{22} as in (40) and $\bar{R}_{12}$ as in (41) and

$$R_{22} = \begin{bmatrix} I_{n_{\mathrm{Pi}_{\mathrm{tree}}}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \Pi_{\mathrm{Pu}_{\mathrm{tree}}} & \Pi_{\mathrm{Pu}_{\mathrm{clpath}}} & 0 & 0 \\ 0 & \Pi_{\mathcal{B}_{\mathrm{De}}} & 0 & 0 & \Pi_{\mathrm{Jc}_{\mathrm{ref}}} & \Pi_{\mathrm{HC}} \end{bmatrix},$$

we obtain the decomposition

$$\begin{bmatrix} I_{n_{\mathrm{De}_c}+n_{\mathrm{Re}_c}} & 0 \\ 0 & L_{22} \end{bmatrix} \hat{F}_{\hat{a},\hat{X}_a} \begin{bmatrix} I_{n_{\mathrm{De}_c}+n_{\mathrm{Re}_c}} & \bar{R}_{12} \\ 0 & R_{22} \end{bmatrix} = \begin{bmatrix} I_{n_{\mathrm{De}_c}+n_{\mathrm{Re}_c}} & 0 \\ * & \hat{N}_{22} \end{bmatrix},$$

with

$$\hat{N}_{22} = \begin{bmatrix} A_{\mathrm{HC},\mathrm{Pi}_{\mathrm{tree}}} & 0 & 0 & 0 & 0 & 0 \\ A_{\mathcal{B}_{\mathrm{De}},\mathrm{Pi}_{\mathrm{tree}}} & G_{\mathcal{B}_{\mathrm{De}}} & 0 & 0 & G^T_{\mathrm{Jc}_{\mathrm{ref}},\mathcal{B}_{\mathrm{De}}} & 0 \\ A_{\mathrm{Jc}_{\mathrm{ref}},\mathrm{Pi}_{\mathrm{tree}}} & G_{\mathrm{Jc}_{\mathrm{ref}},\mathcal{B}_{\mathrm{De}}} & A_{\mathrm{Jc}_{\mathrm{ref}},\mathrm{Pu}_{\mathrm{tree}}} & 0 & G_{\mathrm{Jc}_{\mathrm{ref}}} & 0 \\ 0 & 0 & D^T_{\mathrm{tree,clpath}} & D_{\mathrm{clpath}} & 0 & 0 \\ 0 & 0 & D_{\mathrm{tree}} & D_{\mathrm{tree,clpath}} & A^T_{\mathrm{Jc}_{\mathrm{ref}},\mathrm{Pu}_{\mathrm{tree}}} & 0 \\ \hat{b}_{\mathrm{HC},q_{\mathrm{Pi}_{\mathrm{tree}}}} & A_{\mathrm{HC,Pi}} f_{\mathrm{Pi},p_{\mathcal{B}_{\mathrm{De}}}} & 0 & 0 & A_{\mathrm{HC,Pi}} f_{\mathrm{Pi},p_{\mathrm{diff}}} & A_{\mathrm{HC,Pi}} f_{\mathrm{Pi},p_{\mathrm{HC}}} \end{bmatrix}.$$

Using Assumption 2 and Lemma 2, we obtain $G_{\mathrm{Jc}_{\mathrm{ref}}} = 0$ and $G_{\mathrm{Jc}_{\mathrm{ref}},\mathcal{B}_{\mathrm{De}}} = 0$. Furthermore, using Assumption 3, Lemma 2 and Lemma 4, the diagonal entries of $\hat{N}_{22}$ are non-singular. Hence also $\hat{F}_{\hat{a},\hat{X}_a}$ is non-singular. □

Remark 1 Note that $\bar{N}$ and $\hat{N}$ agree up to their last block rows. The last block row of $\hat{N}$ is given by $F_{\mathrm{HC},\hat{X}_a}$. With $F_{\mathrm{HC}} = Z_{22}^T \dot{F}_a - Z_{22}^T \dot{F}_{a,\dot{X}_d} F_d$, the partial derivative with respect to $\hat{X}_a$ reads

$$F_{\mathrm{HC},\hat{X}_a} = Z_{22}^T \dot{F}_{a,\hat{X}_a} - Z_{22}^T \dot{F}_{a,\dot{X}_d,\hat{X}_a} F_d - Z_{22}^T \dot{F}_{a,\dot{X}_d}, F_{d,\hat{X}_a}.$$

On the other hand, the last block row of $\bar{N}$ is given by

$$Z_{22}^T \dot{F}_{a,\hat{X}_a} - Z_{22}^T \dot{F}_{a,\dot{X}_d} F_{d,\hat{X}_a}.$$

Hence, the last block rows agree if and only if $Z_{22}^T \dot{F}_{a,\dot{X}_d,\hat{X}_a} F_d = 0$.

Combining the concept of derivative arrays [5] and the strangeness index as developed in [11,12, 13,14] with graph theoretical results, the unique solvability of the DAE model (7) can be characterized.

Theorem 1 *Let $\mathcal{N}$ be a network with graph $\mathcal{G}$ and network function $F_{\mathcal{N}}$ that is coupled to a collection of FMUs $\{\mathcal{B}_{De_k}\}_{k=1,\dots,n_{De_c}}$, $\{\mathcal{B}_{Re_k,Pi}\}_{k=1,\dots,n_{Re_c,Pi}}$ and $\{\mathcal{B}_{Re_k,Pu}\}_{k=1,\dots,n_{Re_c,Pu}}$. Let Assumption 1, Assumption 2 and Assumption 3 be satisfied.*

1. *The DAE (7) is regular and has strangeness index $\mu = 1$ (d-index 2).*
2. *The DAE (7) is uniquely solvable for every initial value $(t_0, q_0, p_0, u_0, y_0, x_0) \in \mathcal{C}_{IV}$ and the solution is $(q, p, u, y, x) \in C^1(\mathcal{I}, \mathbb{R}^n)$.*
3. *Given an initial value $(t_0, q_0, p_0, u_0, y_0, x_0) \in \mathcal{C}_{IV}$, a function $(q, p, u, y, x) \in C^1(\mathcal{I}, \mathbb{R}^n)$ solves the DAE (7) if and only if it solves the surrogate model (32).*

Proof We structure the proof in the following way.

(1) Using the concept of the strangeness index and derivative arrays, we derive the surrogate model (32) and show that every solution of the DAE model (7) solves this surrogate model (32).
(2) Vice versa, we show that every solution of the surrogate model (32) solves the DAE model (7).
(3) Transforming the surrogate model (32) to an explicit DAE, whose solvability is covered by the theory of ODEs and by the Implicit Function Theorem, we show that the solution set of the surrogate model (32) is not empty.

Step (1): Given the network function F, cp. (5), and its time derivative $\dot F$, cp. (34), we consider the derivative array [15] $[F^T, \dot F^T]^T$. For the Jacobians

$$N = -\begin{bmatrix} F_X \\ \dot F_X \end{bmatrix}, \quad M = \begin{bmatrix} F_{\dot X} & F_{\ddot X} \\ \dot F_{\dot X} & \dot F_{\ddot X} \end{bmatrix},$$

we show that $\mathrm{rank}(Z_2^T N) = \hat a$ and $\mathrm{rank}(M) + \mathrm{rank}(Z_2^T N) = 2n$ where $\mathrm{span}(Z_2) = \mathrm{coker}(M)$.

With $F_{\dot X} = \dot F_{\ddot X} = \mathrm{diag}\,(I_d, 0)$, $d = n_{\mathrm{St}} + n_{\mathrm{Pi}}$, and $F_{\ddot X} = 0$, there exists a permutation P, such that

$$M = P^T \begin{bmatrix} I_d & 0 & 0 & 0 \\ * & I_d & * & 0 \\ \dot F_{a,\dot X_d} & 0 & \dot F_{a,\dot X_a} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} P,$$

with $\dot F_{a,\dot X_a}$, $\dot F_{a,\dot X_d}$ as in (35), (38). Hence, $\mathrm{rank}(M) = 2d + \mathrm{rank}(\dot F_{a,\dot X_a})$. Under Assumption 2 and Assumption 3, Lemma 7 applies, implying that $\mathrm{rank}(\dot F_{\mathrm{a},\dot X_a}) = a - |\mathcal{C}_{\mathrm{Re},\mathrm{HC}}|$. Then, $\mathrm{rank}(M) = 2d + a - |\mathcal{C}_{\mathrm{Re},\mathrm{HC}}|$. Next, we have to check the rank of $Z_2^T \Pi_{\mathrm{Pi}}^T N$, where $Z_2 \in \mathbb{R}^{2n\times \hat a}$ is such that $\mathrm{span}(Z_2) = \mathrm{coker}(M)$. Considering the Schur complement of M, we find that

$$Z_2^T \Pi_{\mathrm{Pi}}^T = \begin{bmatrix} 0 & 0 & 0 & I_a \\ -Z_{22}^T \dot F_{\mathrm{a},\dot X_d} & 0 & Z_{22}^T & 0 \end{bmatrix}, \tag{44}$$

where $Z_{22} \in \mathbb{R}^{a\times|\mathcal{C}_{\mathrm{Re},\mathrm{HC}}|}$ is such that $\mathrm{span}(Z_{22}) = \mathrm{coker}(\dot F_{a,\dot X_a})$. Then,

$$Z_2^T \Pi_{\mathrm{Pi}}^T N = \begin{bmatrix} F_{\mathrm{a},X} \\ -Z_{22}^T B_{21} F_{\mathrm{d},X} + Z_{22}^T \dot F_{\mathrm{a},X} \end{bmatrix}.$$

Using the representation of Z_{22} given in Lemma 7, we find that $Z_2^T \Pi_{\mathrm{Pi}}^T N = \bar N$ with $\bar N$ given by (39). Under Assumption 2 and Assumption 3, Lemma 8 applies and it follows that $\mathrm{rank}(Z_2^T \Pi_{\mathrm{Pi}}^T N) = \hat a$. Using that $\hat a = a + |\mathcal{C}_{\mathrm{Re},\mathrm{HC}}|$, we thus find that $\mathrm{rank}(M) + \mathrm{rank}(Z_2^T N) = 2n$.

Next, we show the existence of a matrix $Z_1 \in \mathbb{R}^{n\times \hat d}$ with $\mathrm{rank}(Z_1) = \hat d$, such that $\mathrm{rank}(Z_1^T F_{\dot X} T_2) = \hat d$, where the matrix $T_2 \in \mathbb{R}^{n\times \hat d}$ is such that $\mathrm{span}(T_2) = \ker(Z_2^T \Pi_{\mathrm{Pi}}^T N)$. As $F_{\dot X} = \mathrm{diag}\,(I_d, 0)$, we only need the rows of T_2 associated with the differential variables q_{Pi}, x. Using Lemma 8, we thus get

$$F_{\dot X} T_2 = \begin{bmatrix} -\Pi_{\mathrm{Pi}_{\mathrm{tree}}} A_{\mathrm{HC},\mathrm{Pi}_{\mathrm{tree}}}^{-1} g_{\mathrm{HC},x} & \Pi_{\mathrm{Pi}_{\mathrm{chord}}} - \Pi_{\mathrm{Pi}_{\mathrm{tree}}} A_{\mathrm{HC},\mathrm{Pi}_{\mathrm{chord}}} \\ I_{n_{\mathrm{St}}} & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

Choosing

$$Z_1^T = \begin{bmatrix} \Pi_{\mathrm{Pi}_{\mathrm{chord}}}^T & 0 & 0 & 0\,0\,0\,0 \\ 0 & 0 & I_{n_{\mathrm{St}}} & 0\,0\,0\,0 \end{bmatrix}, \tag{45}$$

we find that $Z_1 \in \mathbb{R}^{n\times \hat d}$ satisfies $\mathrm{rank}(Z_1) = \hat d$ as well as $\mathrm{rank}(Z_1^T F_{\dot X} T_2) = \hat d$.

By construction of Z_1, Z_2, a solution of the DAE (7) solves the system

$$\begin{aligned} Z_1^T F(X) &= 0, \\ Z_2^T [F^T, \dot F^T]^T (X) &= 0, \end{aligned}$$

see [15]. With Z_1 given by (45), we verify that $Z_1^T F = [(\Pi_{\mathrm{Pi}_{\mathrm{chord}}}^T F_{\mathrm{Pi}})^T, f_{\mathrm{St}}^T]^T$, i.e., $Z_1^T F = \hat{F}_d$. With Z_2 given by (44), we have

$$Z_2^T \begin{bmatrix} F \\ \dot{F} \end{bmatrix} = \begin{bmatrix} F_a \\ Z_{22}^T \dot{F}_a - Z_{22}^T \dot{F}_{a,\dot{X}_d} F_d \end{bmatrix},$$

where Z_{22} is given by (36). Then,

$$Z_{22}^T \dot{F}_a - Z_{22}^T \dot{F}_{a,\dot{X}_d} F_d = U^T \dot{F}_{\mathrm{HC}} - \Pi_{\mathrm{HC},c}^T \dot{F}_{\mathcal{B}_{\mathrm{De}}} - g_{\mathrm{HC},x} F_{\mathcal{B}_{\mathrm{St}}} - A_{\mathrm{HC,Pi}} F_{\mathrm{Pi}},$$

and inserting $F_{\mathcal{B}_{\mathrm{St}}}$, F_{Pi} from (5) and $\dot{F}_{\mathcal{B}_{\mathrm{De}}}$, $\dot{F}_{\mathrm{Jc}}$ from (34), we get

$$Z_{22}^T \dot{F}_a - Z_{22}^T \dot{F}_{a,\dot{X}_d} F_d = \dot{g}_{\overline{\mathrm{Jc}_{\mathrm{HC}}}} + A_{\mathrm{HC,Pi}} f_{\mathrm{Pi}} + A_{\mathrm{HC,De}} \dot{\bar{q}}_{\mathrm{De}}.$$

The total time derivative is given by $\dot{g}_{\overline{\mathrm{Jc}_{\mathrm{HC}}}} = g_{\mathrm{HC},p_{\mathrm{Jc}_c}} \dot{p}_{\mathrm{Jc}_c} - g_{\mathrm{HC},x}\dot{x} + g_{\mathrm{HC},t}$. Using that the solution $f_{\mathrm{St}}(t, x, p_{\mathrm{Jc}_c}, q_{\mathrm{Pi}_c}, q_{\mathrm{Pu}_c}) = \dot{x}$ solves the state equations, and noting that $g_{\mathrm{HC},p_{\mathrm{Jc}_c}} = 0$ by the definition of $\mathcal{C}_{\mathrm{Re},\mathrm{HC}}$, cp. (10), we find that $Z_2^T[F^T, \dot{F}^T]^T = [F_a^T, F_{\mathrm{HC}}^T]^T$ with F_{HC} given by (31b). Hence, $Z_2^T[F^T, \dot{F}^T]^T = \hat{F}_{\hat{a}}$.

Thus, every solution of the DAE (7) solves the surrogate model (32). By construction, the surrogate model has strangeness index $\hat{s} = 0$, cp. [15].

Step (2): Now, we show that every solution of the surrogate model (32) also solves the DAE (7). Let X solve (32). To reconstruct the differential equation (6b), we differentiate the mass balance $F_{\mathrm{Jc}}(X) = 0$ and find that X also solves

$$0 = A_{\mathrm{Jc,Pi}} \dot{q}_{\mathrm{Pi}} + A_{\mathrm{Jc,Pu}} \dot{q}_{\mathrm{Pu}} + \dot{y}_{\mathrm{De}} + A_{\mathrm{Jc}_e,\mathrm{De}} \dot{q}_{\mathrm{De}_e}.$$

Multiplying this equation by Π_{HC}^T and using that $A_{\mathrm{HC,Pi}_{\mathrm{tree}}}$ is non-singular, we get

$$\dot{q}_{\mathrm{Pi}_{\mathrm{tree}}} = -A_{\mathrm{HC,Pi}_{\mathrm{tree}}}^{-1} \big(A_{\mathrm{HC,Pi}_{\mathrm{chord}}} \dot{q}_{\mathrm{Pi}_{\mathrm{chord}}} + \dot{y}_{\mathrm{De}} + A_{\mathrm{Jc}_e,\mathrm{De}} \dot{q}_{\mathrm{De}_e}\big).$$

Inserting the differential equation (31a) for $\dot{q}_{\mathrm{Pi}_{\mathrm{chord}}}$, it follows that X solves

$$\dot{q}_{\mathrm{Pi}_{\mathrm{tree}}} = -A_{\mathrm{HC,Pi}_{\mathrm{tree}}}^{-1} \big(A_{\mathrm{HC,Pi}_{\mathrm{chord}}} f_{\mathrm{Pi}_{\mathrm{chord}}} + \dot{y}_{\mathrm{De}} + A_{\mathrm{Jc}_e,\mathrm{De}} \dot{q}_{\mathrm{De}_e}\big).$$

Using that $\Pi_{\mathrm{Pi}_{\mathrm{chord}}} \Pi_{\mathrm{Pi}_{\mathrm{chord}}}^T = I - \Pi_{\mathrm{Pi}_{\mathrm{tree}}} \Pi_{\mathrm{Pi}_{\mathrm{tree}}}^T$ as $[\Pi_{\mathrm{Pi}_{\mathrm{tree}}}, \Pi_{\mathrm{Pi}_{\mathrm{chord}}}]$ is a permutation, we have

$$\begin{aligned} A_{\mathrm{HC,Pi}_{\mathrm{tree}}}^{-1} A_{\mathrm{HC,Pi}_{\mathrm{chord}}} f_{\mathrm{Pi}_{\mathrm{chord}}} &= A_{\mathrm{HC,Pi}_{\mathrm{tree}}}^{-1} (A_{\mathrm{HC,Pi}} f_{\mathrm{Pi}} - A_{\mathrm{HC,Pi}_{\mathrm{tree}}} f_{\mathrm{Pi}_{\mathrm{tree}}}) \\ &= f_{\mathrm{Pi}} - A_{\mathrm{HC,Pi}_{\mathrm{tree}}}^{-1} A_{\mathrm{HC,Pi}_{\mathrm{tree}}} f_{\mathrm{Pi}_{\mathrm{tree}}}. \end{aligned}$$

Differentiating the demand FMU output equation (6e), we further replace $\dot{y}_{\mathrm{De}}$ by $\dot{g}_{\overline{\mathrm{Jc}_{\mathrm{HC}}}}$ and thus get

$$\dot{q}_{\mathrm{Pi}_{\mathrm{tree}}} = f_{\mathrm{Pi}_{\mathrm{tree}}} - A_{\mathrm{HC,Pi}_{\mathrm{tree}}}^{-1} \big(A_{\mathrm{HC,Pi}} f_{\mathrm{Pi}} + \dot{g}_{\overline{\mathrm{Jc}_{\mathrm{HC}}}} + A_{\mathrm{Jc}_e,\mathrm{De}} \dot{q}_{\mathrm{De}_e}\big).$$

However, as X solves the hidden constraints (31b), we have

$$A_{\mathrm{HC,De}} \dot{\bar{q}}_{\mathrm{De}} + \dot{g}_{\overline{\mathrm{Jc}_{\mathrm{HC}}}} + A_{\mathrm{HC,Pi}} f_{\mathrm{Pi}} = 0,$$

implying that X solves

$$\dot{q}_{\mathrm{Pi}_{\mathrm{tree}}} = f_{\mathrm{Pi}_{\mathrm{tree}}}(q_{\mathrm{Pi}_{\mathrm{tree}}}, p_{\mathrm{Jc}}, \bar{p}_{\mathrm{Re}}). \tag{46}$$

Replacing the hidden constraints (31b) by the differential equation (46), it follows that every solution of the surrogate model also solves the original DAE.

Step (3): Using the transformations $\Pi_{F_{\mathrm{Jc}}}$, $\Pi_{F_{\mathrm{Pu}}}$ and Π_{Pi}, we show that the surrogate model can be decoupled to an explicit system, whose unique solvability is covered by classical ODE theory and the Implicit Function Theorem. Given Assumption 2 and Assumption 3, Lemma 9 can be applied, implying that the Jacobian $\hat{F}_{\hat{a},\hat{X}_a}$ is non-singular. By the Implicit Function Theorem, there exists a function $\hat{G}_a$ of the differential components, such that $\hat{F}(\hat{G}_a(\hat{X}_d)) = 0$. Then, the differential equations of (32) read

$$\dot{X}_d = \hat{F}_d(X_d, \hat{G}_a(X_d)). \tag{47}$$

As a combination of linear and Lipschitz continous functions, also $\hat{F}_d(X_d, \hat{G}_a(X_d))$ is Lipschitz continuous, hence equation (47) can be uniquely solved for $\hat{X}_d$. □

8 Example

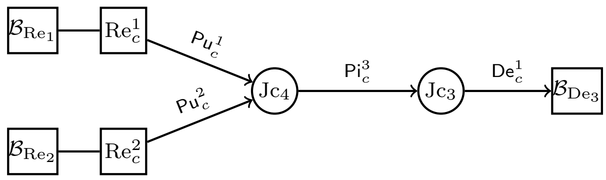


Fig. 3: Graph $\mathcal{G}_{\mathrm{Ex1}}$ of network $\mathcal{N}_{\mathrm{Ex1}}$.

Consider the network given in Figure 3. The network function F of $\mathcal{G}_{\mathrm{Ex1}}$ is given by

$$F = [F_{\mathcal{B}_{\mathrm{St}}}^T, F_{\mathrm{Pi}}^T, F_{\mathrm{Pu}}^T, F_{\mathrm{Jc}}^T, F_{\mathcal{B}_{\mathrm{De}}}^T, F_{\mathcal{B}_{\mathrm{Re,Pu}}}^T]^T,$$

with

$$\begin{aligned}
F_{\mathcal{B}_{\mathrm{St}}} &= \begin{bmatrix} [\dot{x}_i - f_{\mathrm{St}_i}(t, x_i, q_{\mathrm{Pu}_i})]_{i=1,2} \\ \dot{x}_3 - f_{\mathrm{St}_3}(t, x_3, p_{\mathrm{Jc}_3}) \end{bmatrix} \\
F_{\mathrm{Pi}} &= \dot{q}_{\mathrm{Pi}_3} - f_{\mathrm{Pi}_3}(q_{\mathrm{Pi}_3}, p_{\mathrm{Jc}_3}, p_{\mathrm{Jc}_4}) \\
F_{\mathrm{Jc}} &= \begin{bmatrix} q_{\mathrm{Pu}_1} + q_{\mathrm{Pu}_2} - q_{\mathrm{Pi}_3} \\ q_{\mathrm{Pi}_3} - g_{\mathrm{Jc}_3}(t, x_3, p_{\mathrm{Jc}_3}) \end{bmatrix} \\
F_{\mathrm{Pu}} &= [p_{\mathrm{Jc}_4} - g_{\mathrm{Pu}_i} - f_{\mathrm{Pu}_i}(q_{\mathrm{Pu}_i})]_{i=1,2} \\
F_{\mathcal{B}_{\mathrm{Re,Pu}}} &= [y_{\mathrm{Re}_i,\mathrm{Pu}} - g_{\mathrm{Re}_i,\mathrm{Pu}}(t, x_i, q_{\mathrm{Pu}_i})]_{i=1,2} \\
F_{\mathcal{B}_{\mathrm{De}}} &= y_{\mathrm{De}_3} - g_{\mathrm{De}_3}(t, x_3, p_{\mathrm{Jc}_3}).
\end{aligned}$$

The incidence matrix is given by

$$A = \begin{array}{c} \\ \mathrm{Jc}_3 \\ \mathrm{Jc}_4 \\ \mathrm{Re}_1 \\ \mathrm{Re}_2 \end{array} \begin{array}{c} \begin{array}{cccc} q_{\mathrm{Pi}_3} & q_{\mathrm{Pu}_1} & q_{\mathrm{Pu}_2} & q_{\mathrm{De}_3} \end{array} \\ \begin{bmatrix} -1 & 0 & 0 & 1 \\ 1 & -1 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \end{array}.$$

To set up the surrogate model, we identify and classify the maximally connected pump components in $\mathcal{G}_{\mathrm{Ex1}}$. The maximally connected pump components of $\mathcal{G}_{\mathrm{Ex1}}$ are given by $\mathcal{C}_1 = \{\mathrm{Jc}_4, \mathrm{Pu}_1, \mathrm{Pu}_2\}$ and $\mathcal{C}_2 = \{\mathrm{Jc}_3\}$. The component $\mathcal{C}_1$ is connected to two reservoir FMUs, hence $\mathcal{C}_1 = \mathcal{C}_{\mathrm{Re}}$. Conversely, Jc3 is neither connected to a reservoir or reservoir FMU, hence $\mathcal{C}_2 = \mathcal{C}_{\not{\mathrm{Re}}}$.

The component $\mathcal{C}_1$ establishes a closed path, as two reservoir FMUs are connected. The transformation Π_{Pu} is thus given by

$$\Pi_{\mathrm{Pu}_{\mathrm{tree}}} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \Pi_{\mathrm{Pu}_{\mathrm{clpath}}} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

Then, Assumption 3 is satisfied if and only if

$$g_{\mathrm{Re}_1,\mathrm{Pu},q_{\mathrm{Pu}_1}} - f_{\mathrm{Pu}_1,q_{\mathrm{Pu}_1}} + g_{\mathrm{Re}_2,\mathrm{Pu},q_{\mathrm{Pu}_2}} - f_{\mathrm{Pu}_2,q_{\mathrm{Pu}_2}} \neq 0.$$

To verify Assumption 2, we distinguish two cases.

Case 1 Let the demand FMU be input-independent. Then, $\mathcal{C}_2 = \mathcal{C}_{\text{Re},\text{HC}}$ and Assumption 2 is satisfied without any further condition. The matrix selecting the hidden constraints is given by

$$\Pi_{\text{HC}} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

and the vertex identification of $\mathcal{G}_{\text{Ex},1}$ is given by $\overline{\mathcal{JC}}_{\text{HC}} = \{\text{Jc}_4\}$. A spanning tree of $\{\overline{\mathcal{JC}}_{\text{HC}}, \mathcal{PI}\}$ is naturally given by Pi_3.

Then, the surrogate network function is given by $\hat{F} = [F^T_{\mathcal{B}_{\text{St}}}, F^T_{\text{Jc}}, F^T_{\text{Pu}}, \hat{F}^T_{\text{HC}}, F^T_{\mathcal{B}_{\text{De}}}, F^T_{\mathcal{B}_{\text{Re,Pu}}}]^T$ with

$$\hat{F}_{\text{HC}} = \dot{g}_{\text{De}_3}(t, x_3) - f_{\text{Pi}_3}(q_{\text{Pi}_3}, p_{\text{Jc}_3}).$$

Hence, the differential equations for Pi_3 is replaced by the hidden constraints $\hat{F}_{\text{HC}}(X) = 0$. The mass flow q_{Pi_3} is determined by the mass balance.

Case 2 Let the demand FMU be input-dependent. Then, $\mathcal{C}_2 = \mathcal{C}_{\text{Re},\mathcal{B}_{\text{De}}}$. As only one demand FMU is present, Assumption 2 is again satisfied without further conditions on the FMU. As $\mathcal{C}_{\text{Re},\text{HC}} = \emptyset$, no hidden constraints are present, implying that $A_{\text{HC},\text{Pi}}$ is the empty matrix. Hence, Pi_2 is lying on the chord set, i.e., the mass flow q_{Pi_2} is specified differentially. Then, the surrogate network function is given by $\hat{F} = F$.

9 Conclusion and discussion

So far physical networks have been considered mainly as isolated and stand-alone, but in many application they are not. The derivation of physical based topological conditions is also required for coupled systems of physical DAEs with black-box models like FMUs. We have shown, that for coupled DAE-FMU systems easy-to-check topology based rules can be derived. Those rules depend on both, the topology of the physical network and the internal dependency graph of the FMUs. It is quite remarkable, that the conditions for the coupled DAE-FMU networks are a natural extension of the conditions for a stand-alone physical networks. This has the immediate consequence that the surrogate model of the coupled DAE-FMU can be directly assembled from the surrogate model of the DAE and the equations of the FMU without any further manipulations. Indeed, this is a huge benefit and is due to the special design of the FMUs, as well as to the choice or the coupling condition and the underlying analysis.

The main driving feature for the presented approach is the possibility to combine assembled models without changing the models itself (or changing initial conditions). Indeed this feature can not be guaranteed by using purely graph theoretical approaches like Pantelides or the Σ-Method. Anyhow, those algorithms have their right to exists in all applications, where a tight connection to the underlying physics is not relevant or not available. For modular system simulation software the strong connection to the physics increases the applicability in engineering approaches and therefore has to be preferred.

In this work we have considered liquid flow network as a representative example. Indeed, those topics are also relevant for other physical domains like gas–dynamics and electric networks. To the authors best knowledge, the coupling of electrical network and FMUs via defined interface and coupling conditions has not been considered so far. For the *Modified nodal analysis* applied to electric networks, the challenge definitely is hidden in the identification and correct treatment of CV-loops and IL-cutsets, that arise through the coupling procedure. At least the case of CV-loops in electrical networks may be equivalent to the case of pump circles in liquid flow networks.

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