DISSERTATION

IDENTIFICATION OF LINEAR MATERIAL FLOW SYSTEMS - A GRAPH THEORETIC APPROACH

(Identifikation linearer Stofffluss-Systeme)

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KURZFASSUNG


Für Stoffflussmodelle stellen sich die Aufgaben des Messdatenausgleichs, der datengetriebenen Modellierung und der Politiksimulation. In dieser Arbeit werden dazu lineare Modelle für den statischen als auch für den dynamischen Fall vorgestellt. Im statischen Fall sind alle drei Aufgaben in zufriedenstellendem Ausmaß untersucht worden. Prozeduren zur Schätzung von gemessenen und ungemessenen Flüssen, die auf einem allgemeinen Kleinst-Quadrate-Problem basieren, sowie zur Identifikation der Modellparameter werden hier angegeben, Originus Analysis und Fehlerfortpflanzung werden graphentheoretisch untersucht.

Um zu dynamischen Stoffflussmodellen zu gelangen, wird von einer auf einem einfachen Lagerabbaumuster basierenden Modellklasse ausgegangen, die in dem Sinne prototypisch ist, dass eine Reihe von Ergebnissen für kompliziertere Systeme auf jene für den einfachen Fall zurückgeführt werden können. Im Rahmen eines durch die A-priori-Information hoch strukturierten Zustandsraummodells werden auf diese Weise graphentheoretische Lösungen zu Fragen der Stabilität, Erreichbarkeit, Beobachtbarkeit und Identifizierbarkeit gegeben.
ABSTRACT

During the last two decades, Material Flow Analysis (MFA) has become an important instrument in environmental science and pollution research. MFA is a method for capturing, describing and interpreting the metabolism of selected parts of the anthroposphere. Such parts may be regions or production sites in which flows of selected materials, i.e. chemical elements or their compounds, or of goods are measured.

The usual procedure in MFA is to represent a system by a block diagram showing the decomposition of the system into subsystems and the flows between the subsystems, additionally containing the flow measurements. From this flow sheet we directly deduce a system graph, where each vertex represents a subsystem and each (directed) edge a flow. This fact suggests the use of graph theoretic concepts and methods for answering system theoretic questions. In this work it is tried to find an expression and interpretation of, e.g., stability, reachability and identifiability in graph theoretic terms, which, in the consequence, may lead to statements on the material flow level. In other words, we want to decide, whether the underlying material flow system satisfies certain properties, by inspection of the associated system graph.

Here we are concerned with identifying the system from the a priori information and the data. The special features of this system identification problem are: The decomposition into subsystems, the law of the conservation of mass within each subsystem and the positivity of the variables involved, i.e. of the flows and of the levels of the stock within the subsystems. In most applications the stock levels, which often are of great practical interest, are not directly observed. However, there are measurements of import, export and internal flows, but in general in all three flow categories there are unobserved flows as well. Typically, there is only one measurement per balancing period (mostly one year) so that in the static case the balance equations, which equate the sum of the inputs of a subsystem to the sum of its outputs according to the law of the conservation of mass, will be used to reduce the degrees of freedom.

The problems considered for material flow systems are the reconciliation of the flow measurements, data driven modelling and policy simulation. This thesis presents linear models for the static and the dynamic case. In the static case all three tasks have been investigated to a satisfactory degree. Here, we give procedures for the estimation of measured and unmeasured flows, which are based on a generalised least squares problem, and for the identification of the model parameters as well as a graph theoretic treatment of origins analysis and error propagation.

In order to elaborate dynamic material flow models we start from a model class based on a simple stock-building pattern which has a prototype character inasmuch as many results for more sophisticated patterns can be traced back to their analogues for the simple type. In this way we give graph theoretic answers to the questions of stability, reachability, observability and identifiability within the framework of a state space model which is highly structured by the available a priori information.
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CHAPTER I

INTRODUCTION

WER FERTIG IST, DEM IST NICHTS RECHT ZU MACHER,
EIN WERDENDE WIRD IMMER DANKBAR SEIN.
(J. W. V. GOETHE, FAUST I)

The twentieth century, and in particular the second half of it, is marked by an enormous increase in the per capita consumption of energy and materials on the one hand and by an increase of the variety of goods and materials in use on the other hand. Fig. I.1 illustrates this fact by showing the temporal change of the composition of municipal solid waste. First, the overall amount of waste per capita and year has approximately tripped during the observed 65 years. This also indicates that material stocks, be it within buildings or within landfills, might be tomorrow’s resources. Secondly, the composition has shifted, new components like plastics and metals have become more and more significant, the solid waste produced by the inhabitants of industrialised countries is now much more heterogenous. Finally, however, also a change on the material level has taken place, beside the quantitative problem we also have a qualitative one in waste disposal, as is shown in the small figure for heavy metals.

It is easy to imagine that similar considerations can be carried out for other sections of the anthroposphere than the waste management, see [Baccini and Brunner, 1991], [Baccini and Bader, 1996] and [Brunner, 1998]. In order to be able to handle the pollution and resource problems entangled with the indicated developments it is now necessary to come from "end-of-the-pipe" solutions to an integral material management strategy, which tries to understand and, as a consequence, to control the mechanisms driving the metabolism of the anthroposphere. The vision behind such a strategy is a society in sustainable development, i.e. a way of running an economy such that the natural (geogenic) rates of reproduction of resources and of decomposition of pollutants, inter-generational or bio-diversity aspects are taken into account (see, e.g., [Van Den Bergh, 1996]).

In the course of this change in approaching environmental problems caused by human activities, a method called Material Flow Analysis (MFA) was developed (see [Baccini and Brunner, 1991]) which tries to capture the flows and stocks of goods and materials within a selected part of the anthroposphere. A region or production site is described by a system decomposed into subsystems between which there are flows and some of which may contain stocks. By taking measurements of flows and stocks for a given year or for a series of successive years one wants to get a full quantitative picture of the considered part, based on which one can perform additional investigations (such as identifying the main source of a pollutant) and policy simulations. Since some of the flows and most of the stocks cannot
be measured or even assessed by other methods it is necessary to complete the picture by other means. This can be done either by assuming plausible values for some of the model parameters (as is proposed, e.g., in [Baccini and Bader, 1996], where uncertainty in the data is taken into account only a posteriori via error propagation and sensitivity analysis) or by using a data reconciliation procedure on the basis of the available data. Beside estimating the flows and the transfer coefficients (which give the portions of the inputs going to a certain output of a subsystem), in general also the parameters describing the stock behaviour, i.e., the temporal pattern according to which the material leaves the stock once it has entered it, have to be identified.

A crucial feature of this work is that the starting point of nearly all system theoretic considerations is a graph, called the system graph, which is directly deduced from the block diagram common in MFA to describe the interconnections between the subsystems of the considered system (for an example see fig. III.1 and fig. III.2).

This thesis is organised as follows: The next chapter gives a short overview of elementary graph theory and also presents some particular graph theoretic definitions and results which will be needed in the remainder of the work.

In chapter III a more detailed presentation of Material Flow Analysis can be found. Before investigating material flow models in detail a class of models called compartmental models is introduced in chapter IV, which are widely used in physiological studies and show some interesting similarities to the models used here. The most important common feature is the compartmentalisation of a system into subsystems (or compartments). Many results which originally have been developed for compartmental systems will be the basis for our
own investigations in material flow systems. The last section of the same chapter is devoted to clarifying some potential notational conflicts between the involved scientific branches (system theory, graph theory, material flow analysis and compartmental analysis).

Chapter V treats the static modelling of material flow systems. After introducing the model class a data reconciliation and estimation procedure based on a generalised least squares problem is elaborated, resulting in proposition V.6. The investigation of estimators for unmeasured flows leads to graph theoretic identifiability conditions for the static case (proposition V.7). After proposing a procedure for incorporating also noisily measured transfer coefficients, a tool called origins analysis is presented which enables one to detect sets of flows which physically cause a considered flow. The last section of this chapter treats the question in which ways (on the system graph) the uncertainties in the measurements determine the uncertainties in the estimators.

The remainder of the thesis is devoted to the dynamic case. Each of the chapters VI to VIII treats a model class able to describe dynamic material flow models with certain stock properties. For the first one it is assumed that each stock has a certain exact residence time (lifetime). After listing and discussing some general conditions which are assumed for this model class, section VI.2 gives important definitions in the context of generic properties and parameterisations. The significance of these definitions is caused by the fact that we are not interested in whether a certain system theoretic property holds for a considered material flow system with particular parameter values, but whether it holds for a given the considered system graph and for all parameter values in the parameter space except on a proper algebraic set. After a thorough presentation of the model class used in the chapter, stability conditions are derived (theorem VI.4). Theorem VI.12 leads to the graph theoretic conditions for reachability (corollary VI.13), alternative conditions are presented in theorem VI.18. Next, we show that the observability conditions are dual to the reachability conditions, even though the (system theoretic) inputs are assumed to be exactly the imports into the whole system while the (system theoretic) outputs may be observed internal and export flows. A section on minimality combines the preceeding results in theorem VI.24. Section VI.6 on identifiability can be called the core of this work. Based on a graph theoretic description of the transfer function of material flow systems we first investigate the occurrence of common factors. The results developed in subsection VI.6.3 finally lead to the main theorem VI.4.2 where necessary and sufficient conditions for identifiability are given.

In chapter VII it is shown that, based on proposition VII.1, the conditions for stability and identifiability in the case of normally distributed lifetimes can, at least under some additional assumptions, be traced back to the simple case treated in the preceding chapter. The results are presented in theorems VII.2 and VII.7, respectively. For reachability and observability we give only necessary conditions.

In chapter VIII a model is presented which generalises the simple case of exact lifetimes in another way, so that a geometrically declining pattern can be described. It is easy to see that the results on stability and reachability are not severely affected by this alteration. However, we can, in the last section, give necessary and sufficient graph theoretic conditions only for local identifiability (theorem VIII.4).

In the last chapter we draw some conclusions and make some final remarks.

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CHAPTER II

GRAPH THEORETIC CONCEPTS

In this chapter an overview of the graph theoretic definitions and concepts which will be used in the remainder of this work is given. More details and the corresponding proofs can be found in relevant textbooks as [Berge, 1973], [Chen, 1976], [Diestel, 1996] or [Harary et al., 1965], a few definitions are taken from [Murota, 1987]. Clearly, some definitions and notation had to be adapted or (in particular in the case of the section on open graphs) added in order to fulfill the needs of the following chapters.

II.1 Graphs and Digraphs

A graph is a pair $G = (V, E)$ of disjoint finite sets $V$ and $E \subseteq V \times V$. The elements of $V$ are called vertices (or nodes) of $G$, those of $E$ are its edges. Let each vertex be identified by an index such that $V = \{1, \ldots, |G|\}$. If we allow for multiple edges, which may be denoted by $(i, j)$, and $(i, j)_2$, then $E$ is a multiset (instead of a set) of elements of $V \times V$ and $G$ is called a multigraph. The number of vertices is called the order of the graph and is denoted by $|G|$.

A directed graph or digraph is a multigraph where the elements of $E$ are ordered pairs which are called directed edges. For a directed edge $e = (i, j)$ the vertex $i$ is called the initial (or source) vertex and denoted by $s(e)$ while vertex $j$ is called the terminal vertex and denoted by $t(e)$. In addition $i$ and $j$ are called incident with $e$. Multiple directed edges, i.e. edges with the same initial and the same terminal vertex, are called parallel edges. Two vertices $i$ and $j$ are neighbouring or adjacent if $(i, j) \in E$ or $(j, i) \in E$ holds. For $V' \subseteq V$ let $N(V')$ denote the set of neighbours of $V'$ in $V \setminus V'$ which is a disjoint union of the set $N^-(V')$ of predecessors and the set $N^+(V')$ of successors of $V'$. $V(G)$ and $E(G)$ denote the vertex set and the edge set (or family of edges, respectively) of a considered graph (or multigraph) $G$.

From now on we will always consider directed graphs if not stated otherwise (although one or the other result may also hold for undirected graphs). The (undirected) multigraph corresponding to a (directed) graph, which is also called the shadow of the graph, is obtained by simply ignoring the orientation of each edge.

Two graphs $G = (V, E)$ and $\tilde{G} = (\tilde{V}, \tilde{E})$ are said to be isomorphic if there exists a bijection $f : V \rightarrow \tilde{V}$ such that for all $i, j \in V$ we have $(i, j) \in E$ if and only if $(f(i), f(j)) \in \tilde{E}$ holds, i.e. the incidence relationships are preserved. In most cases it not useful to distinguish between isomorphic graphs.

The line graph associated with a graph $G = (V, E)$ is the graph with vertex set $E$ and an edge from $e_i$ to $e_j$ if and only if $t(e_i) = s(e_j)$ holds.
A graph \( G' = (V', E') \) with \( V' \subseteq V \) and \( E' \subseteq E \) is a subgraph of \( G \), written as \( G \subseteq G' \). Define \( V(G') = V' \) and \( E(G') = E' \). A subgraph is called induced or spanned by \( V' \subseteq V \) and denoted by \( G_{|V'} \) if \( E' \) contains all edges \((i, j)\) with \( i, j \in V' \). If, in addition, \( E' \) also contains all edges \((i, j)\) with either \( i \in V' \) or \( j \in V' \) then \( G' \) is called the open subgraph induced by \( V' \) and denoted by \( G_{|V'}^* \) (see section II.2). A subgraph \( G' \subseteq G \) is said to cover \( V \) if \( V(G') = V(G) \). The edge boundary of \( G' \) is defined as the family of edges with initial vertex in \( V' \) and terminal vertex in \( V \setminus V' \) or vice versa.

A directed sequence of length \( l \) from \( i_0 \) to \( i_l \) in \( G \) is a subgraph of the form \((V', E')\) with

\[
V' = \{i_0, i_1, \ldots, i_l\} \quad \text{and} \quad E' = \{(i_0, i_1), (i_1, i_2), \ldots, (i_{l-1}, i_l)\}.
\]

If the \( i_k, k = 0, \ldots, l \) are pairwise different, then \((V', E')\) is called a directed path of length \( l \). The length of a path is thus equal to the number of the involved edges so that a path of length \( l \) covers \( l + 1 \) vertices. A path from a vertex \( i \) to itself, i.e. \( V' = \{i\} \) and \( E' = \emptyset \), is per definition of zero length. Adding to a sequence of length \( l - 1 \) the edge \((i_{l-1}, i_0)\) gives a directed (multiple) cycle of length \( l \), while a directed simple cycle is constructed in the same way from a path. Thus the only cyclic subgraph of a simple cycle \( G' \) is \( G' \) itself.

In the definition of a semicycle and of a semipath each edge \((i_k, i_{k+1})\) may also be replaced by \((i_{k+1}, i_k)\), a strict semicycle is a semicycle which is not a directed cycle\(^1\). It is common that a sequence, a path and a cycle in a digraph always denote a directed sequence, a directed path or a directed cycle, respectively, while in an undirected (multi)graph using the simple notion of a sequence, a path or a cycle, respectively, will not cause any confusion. By a loop we mean a cycle of length one. For a vertex \( i_k \) in a path or in a simple cycle \( i_k, i_{k+1} \) and \( i_{k+1} \) are called the successor and the predecessor of \( i_k \), respectively, in the considered path or cycle.

An undirected graph \((V, E)\) is called (weakly) connected if for all vertices \( i \neq j \) there exists a path between \( i \) and \( j \). A digraph is called strongly connected if for all \( i \neq j \) there exist a path from \( i \) to \( j \) as well as one from \( j \) to \( i \). A maximal (weakly) connected non-empty subgraph of the undirected multigraph corresponding to \( G \) or, in the case that \( G \) is an undirected graph, of \( G \) is called a (weak) component of \( G \). In the sense of this definition we may also call a digraph connected if it consists of only one component. A strong component of a digraph \( G \) is a maximal strongly connected non-empty subgraph of \( G \). Note that the property of strong connectedness defines an equivalence relation on \( V \) if each vertex is defined to be strongly connected to itself. In addition a partial order \( \prec \) can be defined on the family of strong components or, equivalently, on the family of the corresponding disjoint subsets \( V_k \) of \( V \) by\(^2\)

\[
V_j \prec V_k \iff \exists j \in V_j, i_k \in V_k : (i_k, i_j) \in E.
\]

The decomposition of a graph into the family \( \{G_{|V_k}, k = 1, \ldots, r\} \) of its \( r \) strong components is unique and will be called the \( S \)-decomposition of the graph.

For a partition \( \{V_1, V_2\} \) of the vertex set of \( G \) the set of edges between \( V_1 \) and \( V_2 \) is called a cut in \( G \). A cutset is a minimal collection of edges the removal of which increases the number of connected components exactly by one. A cut is thus an edge-disjoint union of cutsets. By a positive cutset we mean a cutset where all edges between the produced vertex sets \( V_1 \) and \( V_2 \) have the same direction (cf. the definition of a coarcircuit in [Berge, 1973]). The set of

\(^1\)Berge, 1973 uses the term circuit for a directed cycle, while a cycle in his notation is what we call a semicycle. Other authors use the term directed circuit.

\(^2\)Of course, the hierarchy in this definition may well be reversed.
Graph Theoretic Concepts

II.2 Open Graphs

edges incident with a single vertex is called an incidence cut. Note that a cut and a cycle always have an even number of edges in common.

For a graph \( G = (V, E) \) let \( \{V_k, k = 1, \ldots, r\} \) be any partition of \( V \) and construct a graph \( \tilde{G} = (\tilde{V}, \tilde{E}) \) where each vertex in \( \tilde{V} \) represents one \( V_k \) and with an edge from \( V_k \) to \( V_i \) for each \( (i, j) \in V_k \times V_i \). Then \( \tilde{G} \) is the contraction of \( G \) with respect to the considered partition of \( V \). Note that the process of contraction may produce (new) parallel edges. If parallel edges are deleted the resulting graph is called the condensation of \( G \) with respect to the given partition. The contraction of a graph with respect to its S-decomposition obviously contains no cycles (but will in general contain semicycles).

An undirected graph is called a tree if it is connected and contains no cycles. We will also in the case of digraphs refer to a connected graph which contains no semicycles as a tree. A spanning tree of \( G \) is a subgraph which is a tree and which covers all vertices of \( G \).

A generalised cycle of length \( l \) is a subgraph the components of which are simple cycles where the lengths of these cycles sum up to \( l \). A generalised path of length \( l \) from vertex \( i \) to vertex \( j \) is a subgraph consisting of a path from \( i \) to \( j \) of length, say, \( l_1 \leq l \) and a vertex-disjoint generalised cycle of length \( l - l_1 \). Note that a generalised cycle which is spanning has length \( m \) while a spanning generalised path has length \( m - 1 \).

In a weighted digraph to each edge \( e = (i, j) \) a weight \( t_{ji} \) is assigned. To each cycle of length \( l \) on \( G \) with vertices \( i_1, \ldots, i_l \) the weight

\[
c_{i_1, \ldots, i_l} = (-1)^{l+1} t_{i_1i_2} t_{i_2i_3} \cdots t_{i_li_1}
\]

is assigned. Also to each path of length \( l \) with vertices \( i_0, i_1, \ldots, i_l \) assign the weight

\[
p_{i_0, \ldots, i_l} = (-1)^{l+1} t_{i_0i_1} t_{i_1i_2} \cdots t_{i_{l-1}i_l}.
\]

For each path of zero length we define the weight to be equal to one. The weights assigned to generalised cycles and paths are the products of the weights assigned to the respective components (cycles, paths). The sign of this weight is thus determined by the overall length and the number of components.

Consider the subgraph \( G' \subseteq G \) induced by the vertex set \( V' \subseteq V \). Then the form of order \( l \) on \( V' \) is defined as the sum of the weights of all generalised cycles of length \( l \) on \( G' \) and is denoted by \( \varphi_V^{(l)} \) (see [Audoly and D'Angio, 1983]). The reduced form of order \( l \) for the ordered pair \( (i, j) \) is defined as the sum of the weights of all generalised paths of length \( l \) from \( i \) to \( j \) and is denoted by \( \rho_{ji}^{(l)} \). If not stated otherwise, the reduced forms will refer to the whole vertex set \( V \).

II.2 Open Graphs

It is sometimes convenient to distinguish a certain vertex from the other vertices and consider it as the surrounding vertex, which is also called the reference node or the infinite vertex. This vertex will be referred to by the index 0. It is not taken as an element of \( V \) and will not be counted in \( |G| \). Usually it is not represented in a graphical representation of the graph.

Such a graph may be called open if each component of \( G_{\{V\}} \) is adjacent to vertex 0 in \( G^0 \). Since thus \( G \) (as a usual graph) is by definition always connected we define a connected open

\[ ^3 \text{The graph is then comparable to a network where the source and the sink are identical and the capacities of all edges are infinite.} \]
graph as an open graph where \( G_V \) is connected. Similarly the (strong) components of an open graph are defined as the (strong) components of \( G_V \). Note that a subgraph of an open graph need not be open. We have, however, the following result about the contraction of an open graph which is understood as the contraction with respect to a partition of \( V \cup \{0\} \).

II.1 Lemma

The contraction of an open graph is open.

Proof: Let \( \{V_0, V_1, \ldots, V_r\} \) be a partition of \( V \cup \{0\} \) and assume, without loss of generality, that the surrounding vertex is contained in \( V_0 \). Let \( \tilde{G} \) be the contraction of \( G \) with respect to this partition so that each \( V_k \) corresponds to \( v_k \), say, in the contracted graph. Suppose that there is a component of \( \tilde{G} \), consisting of the vertices \( v_{k_1}, \ldots, v_{k_l} \), which is not adjacent to \( v_0 \). This, however, means that no element of

\[
C = \bigcup_{j=1}^{l} V_{k_j}
\]

is adjacent to the vertex 0 in \( \tilde{G} \). Since by construction \( C \) must be a component of the open graph \( G \), we have a contradiction. \( \Box \)

All edges \((0,j)\) may be called the inputs and all edges \((i,0)\) the outputs of the graph. Note, however, that in a system theoretic context the inputs and outputs will in general not be identical with the inputs and outputs, respectively, according to this graph theoretic definition. In order to avoid confusion we adopt the convention from SFA to call the edges \((0,j)\) and \((i,0)\) the imports (or physical inputs) and exports (or physical outputs), respectively, of the considered graph, while an input or output means a system theoretic input or output, respectively. Parallel imports and parallel exports thus are imports into or exports from the same vertex, respectively. While an edge entering or leaving vertex \( i \) could also be called an import or export, respectively, of the subgraph, which consists only of vertex \( i \), we will use the notions inflow and outflow, respectively, from compartmental analysis.

An (input) stem in an open graph is a path starting at the target of an import, an output stem is a path terminating at the source of an output. For the case where the inputs are identical with the imports, an open graph is called input-connectable if for all \( j = 1, \ldots, |G| \) there exists a path from 0 to \( j \). If \( E^- \subseteq E \) is the set of system theoretic outputs, the graph will be called output-connectable if for all \( i = 1, \ldots, |G| \) there exists a \( k = t(e) \), which may be different from zero, for an \( e \in E^- \) and a path from \( i \) to \( k \).

A trap or a sink in an open graph is a strong component which has no outflow to the rest of the system nor to the surrounding vertex.

II.3 Bipartite Graphs

A bipartite graph \( G = (V,E) \) is defined as a directed graph where \( V \) is partitioned into two disjoint subsets \( V^+ \) and \( V^- \) and where all edges are directed from \( V^+ \) to \( V^- \). A matching on \( G \) is a subset \( E_M \subseteq E \) such that no two edges in \( E_M \) share a common vertex incident with them. A matching of maximal cardinality is called a maximum matching. \( E_M \) is a matching of \( V' \subseteq V \) if each vertex in \( V' \) is incident with an edge in the matching \( E_M \).

We can now formulate the famous Königs-Hall Theorem:

II.2 Theorem

\( \tilde{G} \) contains a matching of \( V^+ \) if and only if \( |N(V')| \geq |V'| \) holds for all \( V' \subseteq V^+ \).
If we add \( d \) vertices to \( V^- \) and connect each of them with all vertices in \( V^+ \) then, according to the theorem, the new graph contains a matching of \( V^+ \) and at least \( |V^+| - d \) edges of this matching are edges of the original graph \( G \). Thus we have:

II.3 **Corollary**

If \( |N(V')| \geq |V'| - d \) holds for all \( V' \subseteq V^+ \) for a given \( d \in \mathbb{N} \) then \( G \) contains a matching of cardinality \( |V^+| - d \).

A bipartite graph may be represented by a matrix where the rows and columns correspond to the elements of \( V^+ \) and \( V^- \), respectively, and with a non-zero element at the \((i,j)\) position exactly if there is an edge from \( i \in V^+ \) to \( j \in V^- \).

II.4 **Matrices and Digraphs**

Consider a digraph \( G = (V, E) \) with \( m = |V| \) and \( n = |E| \) and where the edges are enumerated as \( E = \{e_1, \ldots, e_n\} \). The incidence matrix \( A(G) \) of \( G \) is the \( m \times n \) matrix with elements \( a_{ij} \) given in the following way: for each \( j = 1, \ldots, n \) the only non-zero elements in the \( j \)-th column are \( a_{i1} = -1 \) and \( a_{i2} = +1 \) for \( e_j = (i_1, i_2) \). For an undirected (multi)graph also \( a_{i1} = +1 \).

II.4 **Lemma**

For a graph \( G \) with \( c \) components

\[
\text{rank}(A(G)) = m - c,
\]

holds.

The rank of the incidence matrix of a connected graph therefore equals \( m - 1 \).

For an open digraph there is no row in \( A(G) \) corresponding to the surrounding vertex. Therefore two special cases have to be considered: an import \( e_j = (i_1, i_2) \) gives as the only non-zero element in the \( j \)-th column \( a_{i1} = +1 \) while an export \( e_j = (i_1, 0) \) gives \( a_{i1} = -1 \) as the only non-zero element in the \( j \)-th column. From the definitions given for open graphs we can conclude:

II.5 **Corollary**

For an open graph \( G \) we have

\[
\text{rank}(A(G)) = m,
\]

independently of the number of its components.

For the definition of the cut and the semicycle matrices let us define an orientation for each cut by ordering the associated partition \( \{V_1, V_2\} \) and for a semicycle by a cyclic ordering of the vertices along the semicycle. Furthermore let us assume an arbitrary but fixed ordering for the cuts in \( G \) as well as one for the semicycles. The cut matrix \( C(G) \) is the \((2^{m-c}-1) \times n\) matrix with elements \( c_{ij} \) given as: \( c_{ij} = 0 \) if the edge \( e_j \) is not in the \( i \)-th cut and \( c_{ij} = \pm 1 \) otherwise, where the sign is determined by whether the orientation of the considered cut and edge coincide or not.

Quite analogously we define the semicycle matrix \( S(G) \) as the matrix with elements \( s_{ij} \), \( n \) columns and as many rows as there are semicycles in \( G \). \( s_{ij} = 0 \) holds if the edge \( e_j \) is not in the \( i \)-th semicycle and \( s_{ij} = \pm 1 \) otherwise, where the sign is determined by whether the orientation of the considered semicycle and edge coincide or not.
The subspaces spanned by the rows of \(C(G)\) and of \(S(G)\) are called the \textit{cut space} and the \textit{semicycle space}, respectively. The following lemma summarises some results concerning the above mentioned matrices.

\textbf{II.6 \textbf{Lemma}}

1. For a graph \(G\) with \(c\) components the ranks of \(C(G)\) and \(S(G)\) equal \(m - c\) and \(n - m + c\), respectively. For an open graph these ranks equal \(m\) and \(n - m\), respectively, independently of the number of its components.

2. The incidence matrix is formed by those rows of \(C(G)\) which correspond to the incidence cuts of \(G\). Any \(m - 1\) incidence cuts form a basis of the cut space.

3. The cut space and the semicycle space are orthogonal complements, so that \(C(G)S(G)' = 0\) holds, i.e. the semicycles generate the kernel of the incidence matrix.

\textit{Remark:} For the undirected case [Diestel, 1996] gives an exact algebraic treatment of cut and cycle spaces based on the vertex space \(V(G)\) which is the vector space of all functions from \(V(G)\) to the field with only elements zero and one. There is a natural correspondence between subsets \(V' \subseteq V(G)\) and the indicator function in \(V(G)\) which assigns the value one to all vertices in \(V'\) and zeroes else. The edge space is defined analogously. In a similar manner it is possible to investigate cut and semicycle spaces for directed graphs. <

If a major submatrix of an \(m \times n\) matrix of rank \(m\) denotes a non-singular submatrix of order \(m\) we can formulate

\textbf{II.7 \textbf{Lemma}}

\textit{A square submatrix of the incidence matrix of a connected graph \(G\) is a major submatrix if and only if the columns of this submatrix correspond to the edges of a spanning tree of \(G\).}

The \textit{adjacency matrix} \(B(G)\) corresponding to a weighted graph \(G\) is defined as the \(m \times m\) matrix with elements \(b_{ji}\) given by

\[
b_{ji} = \begin{cases} t_{ji} & \text{for } (i, j) \in E \\ 0 & \text{else} \end{cases}
\]

The adjacency matrix of a non-weighted graph is constructed in same way with the convention that in this case for all \((i, j) \in E\) we have \(t_{ji} = 1\). The graph of order \(m\) corresponding to an \(m \times m\) matrix in the converse manner is called the associated \textit{Coates graph}. The following result is based on the fact that there is a one-to-one correspondence between the non-vanishing terms in

\[
\det(B) = \sum_{\pi} \pm b_{\pi(1)} \cdots b_{\pi(m)}
\]

where the sum is taken over all permutations \(\pi\), and the generalised cycles of length \(m\) on the associated Coates graph.

\textbf{II.8 \textbf{Lemma}}

\textit{Let \(B\) be an \(m \times m\) matrix and \(G\) the associated Coates graph. Then the determinant of \(B\) and the \((t, s)\)-element \(B_{ts}\) of its cofactor matrix can be expressed as}

\[
\det(B) = (-1)^{m} \sum_{c(m)} (-1)^{\gamma(c(m))} \omega(c(m))
\]

(II.2)
\[ B_{tt} = (-1)^{m-1} \sum_{c(m-1)} (-1)^{\gamma(c(m-1))} \omega(c(m-1)) \]  
\[ \text{(II.3)} \]

and for \( s \neq t \)

\[ B_{ts} = (-1)^{m-1} \sum_{p(m)} (-1)^{\gamma(p(m))} \omega(p(m)), \]  
\[ \text{(II.4)} \]

where the sum in (II.2) is taken over all generalised cycles \( c(m) \) of length \( m \) on \( G \), the sum in (II.3) over all generalised cycles of length \( m - 1 \) on \( G \) which do not involve the vertex \( i \) and the sum in (II.4) over all generalised paths \( p(m) \) from \( t \) to \( s \) of length \( m \) on \( G \); \( \omega(.) \) and \( \gamma(.) \) denote the weight of and the number of cycles in the considered generalised cycle or path.

Remark: Note that according to the definition of a path of zero length \( \tilde{B}_{tt} \) may also be expressed as in (II.4) for \( s = t \). <

A matrix \( B \in \mathbb{R}^{m \times m} \) is reducible if there exists an \( m \times m \) permutation matrix \( P \) such that

\[ P^t BP = \begin{pmatrix} B_{11}^* & B_{12}^* \\ 0 & B_{22}^* \end{pmatrix} \]  
\[ \text{(II.5)} \]

where \( B_{11}^* \) and \( B_{22}^* \) are square. \( B \) is called irreducible if it is not reducible. In particular a \( 1 \times 1 \) matrix is irreducible if and only if it contains a non-zero element.

II.9 Lemma

If \( B \in \mathbb{R}^{m \times m} \) is reducible then there exists a permutation matrix \( P \) such that

\[ P^t BP = \begin{pmatrix} B_{11} & B_{12} & \cdots & B_{1r} \\ 0 & B_{22} & \cdots & 0 \\ \vdots & 0 & \ddots & \vdots \\ 0 & 0 & \cdots & B_{rr} \end{pmatrix} \]  
\[ \text{(II.6)} \]

where the \( B_{ii} \) (\( i = 1, \ldots, r \)) are irreducible or scalar zeros.

Proof: If \( B \) is reducible then after permuting its rows and columns accordingly it is partitioned as given in (II.5). Now consider the first diagonal block \( B_{11}^* \). If it is irreducible go on to the second diagonal block \( B_{22}^* \), otherwise it can be transformed by a permutation matrix to be again partitioned as (II.5). This procedure ends when the upper left block of such a submatrix is either irreducible or a scalar zero. Then go back one step in the recursion and proceed as before with the next diagonal block. \( \Box \)

II.10 Corollary

In the Coates graph associated to a square matrix \( B \) as given in (II.6) the strong components exactly correspond to the irreducible diagonal blocks \( B_{ii} \).
CHAPTER III

MATERIAL FLOW ANALYSIS

Societies with a high per capita consumption of energy and materials show a great variety of materials, goods and processes which are used for the satisfaction of human needs. It is estimated that the number of materials involved ranges between $10^4$ and $10^6$, the number of processes is of the same order of magnitude, the number of goods even an order of magnitude higher. Linked to the economic production, consumption and disposal of materials are the problems of resource depletion and emission of hazardous substances into the environment. For the solution of such problems it would therefore in a first step be useful to get a full quantitative (physical) picture of the anthropogenic metabolism, i.e. the material flows and stocks in the anthroposphere.

Material Flow Analysis (MFA) or Substance Flow Analysis has become an important instrument in environmental science and pollution research. It gives a method for capturing, describing and interpreting the metabolism of selected parts of the anthroposphere. Such parts may be regions (i.e. towns, districts, nations, the EU, see [Brunner, 1998]) or production sites, in which flows of selected materials (i.e. chemical elements or their compounds) or goods are measured. One of the earliest references in this area is probably [Ayres, 1978]. According to [Van der Voet et al., 1995b], where also a good overview of existing literature is given, a material flow study comprises three steps: (i) the definition of the system, (ii) the quantification of the overview of stocks and flows and (iii) the interpretation of the results.

The first step, which is often called system analysis ([Baccini and Brunner, 1991], [Baccini and Badar, 1996]) and which we prefer to call verbal modelling, includes (see [Bauer et al., 1997]) the delimitation of the system from the outside world (i.e. the surroundings of the region or of the production site under consideration), the list of the variables (i.e. the flows and stocks), the decomposition into subsystems (in MFA often called processes) and the description of the interconnections between the subsystems. Additional a priori knowledge concerns the subsystems such as (mass) balance equations which are based on the law of the conservation of mass and equate the sum of the inflows of a subsystem to the sum of the outflows of the same subsystem. Sometimes also transfer coefficients are known a priori: If it is assumed that each flow leaving a considered subsystem only depends on the sum of the flows entering it, these coefficients give the portions of the sum of the inflows (including stock depletion flows) which go to the respective outflows (including stock accumulation flows).

Whenever in this work we speak of transfer coefficients we implicitly assume that this condition is valid. Otherwise we have to consider transfer matrices giving the partitioning of each inflow onto the outflows.
Material Flow Analysis

Figure III.1: A hypothetical example of a flow sheet with three subsystems and six flows. The flow amounts are given as intervals of plausible values. The subsystem "Agriculture" has a stock of 150.0 t in the considered year and a stock accumulation of 2.0 to 5.5 t/a.

Note that the choice of the system boundaries refers not only to space, but also to time. Materials flows are given in mass units per time unit (and often also per capita), material stocks in mass units (per capita). Usually, the time unit is one year which in most cases is in accordance with data availability and also with the formulation of material management policies. Listing the variables of the considered system also includes the choice of the materials to be investigated which depends on the questions to be answered for this system. Considering totalised material levels is useful when the material intensity of an economy is of interest, while particular pollution problems often require the selection of an indicator element or one or more chemical compounds which characterise the system with respect to this problem. In the models presented in the subsequent chapters we will only treat the one-material case, an example for a model with more than one component (taking into account chemical reactions between them) is given in [Crowe et al., 1983].

The verbal modelling step results in a flow sheet which is a block diagram of the following form, see [Baccini and Brunner, 1991]: Each subsystem is represented by a rectangle, each flow by an arrow from the rectangle representing the source subsystem to that representing the terminal subsystem. The (spatial) system boundary is indicated by a dashed rectangle which surrounds the rectangles corresponding to the subsystems within the system. The arrows representing imports (i.e. flows from the surroundings of the system into the system) and exports (i.e. flows leaving the system) cross this boundary line in the respective direction. Each rectangle may contain the name or number, the stock level and the accumulation/depletion flow amount of the subsystem which it represents. In addition each arrow is attached an oval which may contain the name or number and the amount of flowing material (see next step) of the flow which it represents. For an example of a flow sheet see fig. III.1.

The flow sheet leads in a natural way to a graph theoretic description of a material flow system: Each vertex corresponds to a subsystem, each directed edge to a flow. The surroundings of the system are represented by the vertex 0, so that the resulting system graph is an open graph. The graph corresponding to the flow sheet in fig. III.1 is shown in fig. III.2. If transfer coefficients are of interest a weighted graph is given as follows: Each edge corresponding to an internal and export flow is weighted by the associated transfer coefficient and each import by one. The system graph will be the starting point for many system theoretic considerations in the following chapters.
The second step in a material flow study consists of data collection and modelling. Material flow data are calculated from data on flows of goods and on material concentrations of these goods. In addition information on transfer coefficients might be available. In general, there are three sources of data which are of different quality (and of different information about this quality), see [Bauer et al., 1997]: (a) Data from technical measurements (e.g. chemical contents of incineration residues), (b) data from administrative records (e.g. production statistics) and (c) data from other studies (which often requires down-scaling) and expert knowledge. Often only certain statistics (like means and standard deviations) of the underlying flow data, especially of the third category, are available. In the models elaborated in the subsequent chapters by measurements we mean flow data from all three categories. It is important to remark that a broad standardised data base based on appropriate statistical surveying systems is not available at date. Therefore the data collection phase within a material flow study is very time consuming. Incongruous definitions and classifications, highly aggregated, missing, non available or non representative data are common. Measurement errors and incomplete data sets are the reasons for the fact that in practically all cases the flow data are inconsistent in as much as the principle of mass conservation is violated. Imposing this principle provides additional information about the unobserved true flows and thus allows for the improvement of the quality of the estimates and for completing the data set. A static data reconciliation procedure is presented in chapter V. Other approaches to the problems listed above can be found, e.g., in [Van der Voet et al., 1995a] and [Baccini and Bader, 1996].

The last step, the interpretation and presentation of the results of the material flow study, is adressed in this work only by the origins analysis tool for the static case (see section V.3, for a case study see [Gleiß et al., 1998]). Linking the results of the quantification step to evaluation methods yields a basis for environmental policy decisions (see e.g. [Wagner et al., 1998]). This issue is also related to the political and socio-economic sciences, see [Brunner, 1998]. The general objectives mentioned in the cited project report show the potential use of such material flow based tools: Early recognition of future problems of environmental loadings and resource depletion, defining and setting priorities for measures to protect the environment and to use resources more efficiently, analysing and improving these measures and changing from filter or end-of-the-pipe strategies to an efficient regional material management in view of sustainable development (monitoring, early recognition and simulation and evaluation of material control strategies).
CHAPTER IV

COMPARTMENTAL ANALYSIS

In [Jacquez, 1972], which is (also in its more recent edition) one of the main references on
this topic, we find the following definition:

A compartmental system is a system which is made up of a finite number of
macroscopic subsystems, called compartments or pools, each of which is homoge-
neous and well-mixed, and the compartments interact by exchanging material.
There may be inputs from the environment into one or more of the compartments
and there may be outputs (excretions) from one or more compartments into the
environment. [...] The mathematical theory of the behaviour of such systems is
called compartmental analysis or the theory of compartmental systems.

It is important to note that a compartment does not necessarily correspond to a physical
volume. It is rather a hypothetical container comprising some material which is assumed
to be well-stirred so that the spacial dimension within the compartment can be neglected.
Sometimes different compartments even mean amounts of different compounds within the
same tank. [Eisenfeld, 1985] cites Richard Bellman, one of the pioneers in the investigation
of identifiability of compartmental systems, with the following short definition of compart-
mental analysis:

It is to determine what is occurring in one compartment by sampling another.

The mathematical description of compartmental systems is treated in, e.g., [Anderson, 1983],
mental representation" is given as a special case of a class of representations of so called
mass balance systems). For the linear case let $x_i(t), i = 1, \ldots, m$ denote the amount of material
in compartment $i$ at time $t$ (with initial value $x_{0i}$ at time zero) and $f_{ij}(t), i, j = 0, \ldots, m$
(where 0 represents the environment of the system) the mass flow rate from compartment
$j$ to compartment $i$ at time $t$. Then the (mass) balance equations, based on the law of the
conservation of mass, for $i = 1, \ldots, m$ are given as

$$\frac{dx_i(t)}{dt} = f_{0i}(t) + \sum_{j \neq i} (f_{ij}(t) - f_{ji}(t)) - f_{0i}(t), \quad 0 \leq t < \infty, \quad x_i(0) = x_{0i}$$

In many applications it is assumed that the flow rates linearly depend on the amount of
material in its source compartment. This results in

$$\frac{dx_i(t)}{dt} = f_{0i}(t) + \sum_{j \neq i} (t_{ij}x_j(t) - t_{ji}x_i(t)) - t_{0i}x_i(t), \quad 0 \leq t < \infty, \quad x_i(0) = x_{0i}$$
Compartmental Analysis

The rate constants $t_{ij}$, $i \neq j$ are called ( fractional) transfer coefficients and give the fraction of the material in the source compartment $j$ which goes to compartment $i$. If we set

$$t_{ii} = - \sum_{j \neq i} t_{ji} - t_{ii}$$

this leads to the following matrix equation:

$$\dot{x}(t) = Tx(t) + s(t)$$

where $T$ is the $m \times m$ matrix containing the $t_{ij}$, $i, j = 1, \ldots, m$ and $s(t) = (f_{01}(t), \ldots, f_{m0}(t))^T$ contains the inputs from the environment.

In the discrete-time case the balance equations for compartments $i = 1, \ldots, m$ yield

$$x_{i,t+1} - x_{i,t} = f_{i0,t} + \sum_{j \neq i} (t_{ij}x_{j,t} - t_{ji}x_{i,t}) - t_{ii}x_{i,t}, \quad t \in \mathbb{N}_0, \quad x_{i,0} = x_{0i}$$

By setting

$$t_{ii} = 1 - \sum_{j \neq i} t_{ji} - t_{ii}$$

we arrive at a description of the form

$$x_{t+1} = Tx_t + s$$

(IV.1)

The properties of the matrix $T$ occurring in the equation (IV.1) will be of interest in the remainder of this work.

Definition: A matrix $T \in \mathbb{R}^{m \times m}$ is called a continuous-time compartmental matrix if its off-diagonal elements are non-negative and all its column sums are less than or equal to zero. A matrix $T \in \mathbb{R}^{m \times m}$ is called a (discrete-time) compartmental matrix if its elements are non-negative and all its column sums are less than or equal to one.

It is clear that there is an excretion of the $i$-th compartment if and only if the $i$-th column sum is strictly less than zero (in the continuous-time case) or one (in the discrete-time case), respectively. See [Eisenfeld and Mitra, 1995] for an investigation of these kinds of matrices.

In the later chapters we will also need the following definition:

Definition: A trap in a compartmental system is a compartment or a set of compartments from which there are no flows to the environment (surroundings) nor to compartments not contained in the set.

Compartmental models are most commonly used in physiology and pharmacokinetics. For ecosystem compartmental models see [Young, 1993]. To the author’s knowledge the application of methods developed for these models to (dynamic) material flow systems is a novelty, although the compartmental structure of material flow systems is obviously given by their definition. Whereas in the biological and medical applications the compartments may represent organs of some species under study, in MFA they correspond to subsystems of the anthroposphere (one of which, in the extreme case, might also be an aggregate of, e.g., the lungs of all human beings living in the considered region). So in both cases the assumption of well-mixed compartments will most often be rather hypothetical and in neither case do the compartments correspond to physical volumes in general.
There is, however, a difference in the scale of the systems and also in the possibility to perform experiments. Typical questions in the context of physiological compartmental models are (see, e.g., [Brown, 1980]): Where shall I inject the tracer substance and where shall I observe the tracer concentration so that I learn as much as possible about my system? How many compartments describe my system most appropriately and do the compartments of my optimal model have a physiological interpretation (black-box compartmental modelling)? Is it useful to impose a priori the number and the interconnections of the compartments? While the questions of parameter identifiability and estimation are also central in the MFA context (see the following chapters), the input and the inner structure as well as their interpretation is given a priori for MFA systems in the flow sheet, so that experiment design is not an issue in this field. In addition, unlike in MFA, biological compartmental models sometimes deal with bidirectional flows (i.e. whenever there is a flow from one compartment to another there is also one in the reverse direction) which lead to undirected compartmental models, see [Hayakawa et al., 1984].

IV.1 A Note on Notational Conflicts

In this and the preceding chapters we have encountered a series of notions and definitions from system theory, graph theory, material flow analysis and compartmental analysis, some of which address the same thing and, at least more or less, also mean the same thing. It is therefore necessary to settle some possible notational conflicts between these disciplines by giving preference to one of them in each case in order to simplify and clarify the presentation of the results of this work.

Where this causes no confusion we will identify the flow sheet with the associated system graph and therefore also the subsystems (instead of processes or compartments) with the vertices and the flows with the corresponding (directed) edges. In the figures showing system graphs we will, as is common in graph theory, use circles instead of rectangles in order to represent subsystems and neglect the ovals attached to the flows. By inputs and outputs we will always mean the system theoretic ones, while the physical ones will be referred to as imports and exports (instead of excretions), respectively. In order to avoid confusion we use the notions inflows and outflows for what would be called the inputs and outputs of subsystems in system theory (see section II.2). Furthermore we adopt the graph theoretic definition of a trap (instead of a sink), which requires the involved subsystems to be strongly connected.

Concerning the definitions of transfer coefficients in this and the previous chapter we adopt that from MFA because of two reasons: First, this is more appropriate in the static case, where stock accumulation or depletion flows are modelled as export and imports, respectively. Secondly, in the dynamic models we will trace back the considered stock accumulation/depletion patterns to a case where the amount of material leaving the stock is not proportional to the stock level. Moreover, the transfer coefficients of a dynamic subsystem are defined as shown in fig. VI.1.
CHAPTER V

A STATIC MODEL

In this chapter a linear model for the static material flow problem is presented. The results for all except the last section are based on the articles [Bauer et al., 1997] and [Gleiß et al., 1998]. The presentation given here, however, will make more extensive use of the graph theoretic concepts introduced in chapter II. For an approach to non-linear problems of a similar kind see [Crowe, 1986]. Note that, if we consider a dynamic subsystem in the static model, the stock accumulation flows are modeled as exports and the stock depletion flows as imports, the intertemporal information is neglected.

Throughout the whole chapter, the system graph means the graph which corresponds to the flow sheet described in chapter III, i.e. each vertex represents a subsystem and each edge a flow. The system graph is denoted by $G = (V,E)$. From what was said in the Material Flow Analysis chapter we may presume that the system graph is open. In the following we will often not distinguish formally between the edges of the system graph and the associated (true) flows as well as between the vertices and the associated subsystems $1, \ldots, m$.

V.1 The Model Class

Let $f \in \mathbb{R}^n$ be the vector of all true (or latent) flows within the considered material flow system, i.e. the components $f_j$ of $f$ may be imports, internal flows as well as exports. The linear, static, symmetric model we consider here is of the form

$$Mf = 0 \quad \text{(V.1)}$$

where in the matrix

$$M = \begin{pmatrix} A \\ T \\ R \end{pmatrix}$$

the $m \times n$ submatrix $A$ describes the balance equations, the $c \times n$ submatrix $T$ the transfer coefficient equations and the $d \times n$ submatrix $R$ the linearly independent additional linear relations, which do not satisfy a balance equation and which are linearly independent of the previous equations. Note that the relations described by (V.1) are assumed to be deterministic.

---

1. The stock shown in fig. V.1 thus lies outside the system boundary in this case.
The balance equation for the subsystem $k \in \{1, \ldots, m\}$ has the form

$$
\sum_{j: t(f_j) = k} f_j = \sum_{j: n(f_j) = k} f_j
$$

(V.2)

Note that the balance equation for the surrounding vertex would correspond to a row vector which is equal to the sum of all rows of $A$. It is therefore not included.

Each transfer coefficient equation describes an outflow of a subsystem as a linear combination of its inflows. Thus $c$ equals $n$ minus the number of imports (physical inputs into the whole system), while the number of (system theoretic) inputs equals $n - (c + d)$.

While the balance equations and the transfer coefficient equations are directly related to physical subsystems, i.e. subsystems which satisfy a balance equation, and thus to the system graph associated with the system under consideration, the additional linear relations represent restrictions which cannot be expressed as physical subsystems.

**Remark:** It is useful to assume in the static case that each outflow $f_j$ of a subsystem $k$ only depends on the sum of all inflows, i.e.

$$
f_j = t_j \sum_{i: t(f_i) = k} f_i
$$

Otherwise, i.e. in the case where (exact or noisy) detailed information exists on the fraction, $t_{ji}$ say, which is transferred from a single inflow $f_i$ to $f_j$, the subsystem $k$ can be split up into a set of subsystems: one subsystem for each inflow or outflow, respectively, which is addressed by a detailed transfer coefficient, one subsystem receiving the remaining inflows and one releasing the remaining outflows. There are unmeasured flows from each of the, $n_1$ say, inflow subsystems to each of the, $n_2$ say, outflow subsystems so that the detailed transfer coefficients are of the usual kind, i.e. referring to the sum of inflows, in the expanded system\(^2\). Note that the new unmeasured flows form

$$
\sum_{2 \leq q \leq \min(n_1, n_2)} \binom{n_1}{q} \binom{n_2}{q}
$$

simple semicycles. Therefore (see proposition V.7 below) an equal number of detailed transfer coefficients must be known in order to be able to use the information by working with the expanded system. If this is not the case the information has to be ignored and the assumption that the transfer coefficients refer to the sum of all inflows has to be maintained also for the (whole) subsystem $k$. In the following we may therefore assume that each outflow is assigned only one transfer coefficient $t_j$. \(<1

From (V.2) it follows that the transfer coefficients associated with all outflows of a subsystem $k$ sum up to one, i.e.

$$
\sum_{j: n(f_j) = k} t_j = 1
$$

(V.3)

**V.1 Lemma**

1. For the matrices defined above we have

$$
\text{rank} \begin{pmatrix} A \\ T \end{pmatrix} = \text{rank}(T)
$$

\(^2\)As a special case a detailed zero transfer coefficient i.e. the information that a certain inflow does not transfer material to $f_j$, can be incorporated by deleting the corresponding new unmeasured flow.
2. **The matrix \( A \) has full row rank.**

3. **For a system without traps the matrix \( \begin{pmatrix} T & R \end{pmatrix} \) has full row rank.**

**Proof:** The first statement follows immediately from the fact that the rows of \( T \) associated with all outflows of a subsystem \( k \) sum up to the \( k \)-th balance equation, cf. (V.3). The second statement is a direct consequence of corollary II.5 since we presumed that the system graph is open. For the last one note that by definition the rows of \( R \) are linearly independent of those of \( T \). Thus it remains to show that \( T \) has full row rank. For this purpose let \( T \) (and thus also \( f \)) be partitioned, without loss of generality, into \( (T_1, T_2) \) where \( T_1 \) corresponds to the imports while \( T_2 \) corresponds to the internal and export flows of the system. Furthermore let the rows of \( T \) be arranged such that its \( i \)-th row describes the \( i \)-th internal or export flow, i.e. flow \( f_{n\cdot -i} \), as a function of the relevant inflows. Then the \( n \times n \) matrix \( D \) given as

\[
D = \begin{pmatrix} 0 & 0 \\ T_1 & I + T_2 \end{pmatrix},
\]

where the north-western zero submatrix is quadratic, is a compartmental matrix (see chapter IV) because of (V.3). \( D \) is the adjacency matrix of the linegraph associated with \( G \) and it is clear that there the traps in this graph are in a one-to-one correspondence with the traps in \( G \). Therefore, by theorem VI.4, in the absence of traps the matrix \( D \) is asymptotically stable so that \( I - D \) is regular which shows that \( T_2 \) is regular as well. □

In general neither the matrix \( M \) nor all true flow values are known a priori. For the formulation of the flow measurement model we assume the following partitioning of \( f \):

\[
f = \begin{pmatrix} z \\ x \\ y \end{pmatrix},
\]

where \( z \in \mathbb{R}^n_z \) denotes the subvector of flows with exact (i.e. noisefree) measurement values, \( x \in \mathbb{R}^n_x \) the subvector of flows with noisy measurements \( x^* \) and \( y \in \mathbb{R}^n_y \) the subvector of unmeasured flows. Accordingly, let \( A \) be partitioned columnwise into \( (A_z A_x A_y) \), using an obvious notation. Furthermore it is assumed without loss of generality, that there are no equations in (V.1) which involve only exactly known flows since these equations would give no restrictions on the estimates and could thus be ignored in the reconciliation procedure below. For the noisy measurements we assume that the measurement error \( u = x^* - x \) is normally distributed with zero mean and known variance-covariance matrix \( \Sigma \) which in most cases will be diagonal.

In the same way transfer coefficients, which are elements of \( T \), can be measured with or without noise or be unobserved, which gives a partitioning of the vector \( t \) of transfer coefficients into exactly known, noisyly measured and unmeasured coefficients \( t_e, t_m \) and \( t_u \), respectively. For noisy measurements \( t_{m,j} \) we assume that the measurement error \( v_j = t_{m,j} - t_{m,j} \) for each such transfer coefficient is normally distributed with zero mean and known variance \( \tau_j \). In addition the errors associated with transfer coefficients are assumed independent of each other (so that \( \Omega = Var(t_m) \) is diagonal) and of the flow measurements. The additional linear relations are assumed to be a priori known.
V.2 Data Reconciliation and Estimation

The a priori information which can be exploited in order to improve the data precision consists of the balance equations, those transfer coefficient equations which contain only observed coefficients and the additional linear relations. Let \( \hat{T} \) denote those, \( \hat{\theta} \) say, rows of \( T \) which correspond to the known transfer coefficient equations and set

\[
\hat{M} = \begin{pmatrix} A \\ \hat{T} \\ R \end{pmatrix}
\]

In addition assume that this matrix has full row rank which means that redundant transfer coefficient equations are ignored. Then, without loss of generality, the matrix \( \hat{M} \) has the following partitioning:

\[
\hat{M} = \begin{pmatrix} \hat{M}_{1z} & \hat{M}_{1z} & 0 \\ \hat{M}_{2z} & \hat{M}_{2z} & \hat{M}_{2y} \end{pmatrix}
\]

where the block columns correspond to exactly known, measured and unmeasured flows. The first block row represents equations which do not involve unmeasured flows. Let the matrices \( A, \hat{T} \) and \( R \) be partitioned in the same way, using an analogous notation. Note that all submatrices in (V.4) may contain coefficients \( t_{m,j} \) for which only noisy measurements exist.

The flow and transfer coefficient measurements are reconciled by solving the following minimisation problem:

\[
\min_{\hat{z}, \hat{\theta}, t_m} (\hat{\theta} - \theta^*)' \Sigma^{-1} (\hat{\theta} - \theta^*) + (\hat{t}_m - t_m^*)' \Omega^{-1} (\hat{t}_m - t_m^*)
\]

w.r.t.

\[
\hat{M} \hat{f} = 0
\]

where we set

\[
\hat{f} = \begin{pmatrix} \hat{z} \\ \hat{x} \end{pmatrix}
\]

and \( \hat{z} = z \). In the case of no unmeasured flows and no measured transfer coefficients the problem (V.5), (V.6) simplifies to

\[
\min_{\hat{z}} (\hat{z} - \theta^*)' \Sigma^{-1} (\hat{z} - \theta^*)
\]

w.r.t.

\[
\hat{M}_{1z} z + \hat{M}_{1z} \hat{z} = 0
\]

where now the matrices involved in the restriction (V.8) contain only a priori known coefficients. This, however, is a General Least Squares (GLS) problem, where the vector of flow measurements is projected onto the right kernel of \( \hat{M} \). The solution

\[
\hat{z} = x^* - \Sigma \hat{M}_{1z}^T (\hat{M}_{1z} \Sigma \hat{M}_{1z}^T)^{-1} (\hat{M}_{1z} x^* + \hat{M}_{1z} z)
\]

is given by the method of Lagrangian multipliers. Note that this solution exists for positive definite \( \Sigma \). Its uniqueness follows from lemma V.1. While [Svenek, 1964] was one of the first to derive this result for the case \( M = A \) and \( f = x \), [Crowe et al., 1983] also allowed for exactly known flows.

By GLS theory (see, e.g., [Schönfeld, 1969]) the solution (V.9) gives efficient estimates \( \hat{x} \), i.e. estimators with minimal variance among all unbiased estimators. Note that for the case \( \hat{M}_{1z} z \neq 0 \) the condition (V.8) restricts the estimates to an affine rather than to a linear subspace.
V.2.1 The Reduced Balance Scheme

If we allow for unmeasured flows to exist in the system under consideration, but still exclude transfer coefficients with noisy measurements the minimisation problem has the following form:

\[
\begin{align*}
\min_{\hat{x}, \hat{\beta}} & \quad (\hat{x} - x^*)'\Sigma^{-1}(\hat{x} - x^*) \\
\text{w.r.t.} & \quad \tilde{M}\hat{f} = 0
\end{align*}
\]  

(V.10) (V.11)

where all submatrices as given in (V.4) exist in general and contain only a priori known coefficients. It is important to see that this problem can no longer be interpreted as a GLS problem since the subvector \( y^* \) of the unknowns is not involved in the objective function.

In order to construct a reduced system graph which again leads to a problem of the kind (V.7), (V.8) we need some definitions:

**DEFINITION:** Those subsystems which are incident with unmeasured flows are called *unmeasured subsystems*. The set of vertices associated with these subsystems is denoted by \( V_2 \subseteq V \). A subsystem which is not unmeasured is called a *measured subsystem*. Set \( V_1 = V \setminus V_2 \).

It follows that the rows of \( \tilde{M} \) representing the balance equations corresponding to unmeasured subsystems belong to the second block row of (V.4).

**V.2 LEMMA**

Consider the (non-open) subgraph \((V \cup \{0\}, E_y)\) of the graph \((V \cup \{0\}, E)\), where \( E_y \) denotes the set of edges associated with unmeasured flows. Then there are exactly three kinds of components:

1. The component, \( U_0 \) say, containing the surrounding vertex.
2. The components, \( \{U_1, \ldots, U_K\} \) say, with order greater than one and not containing the surrounding vertex.
3. The components \( \{v\}, v \in V_1 \).

**DEFINITION:** The partition

\[
\{\{v\}, v \in V_1\} \cup \{U_0, \ldots, U_K\}
\]

of \( V \) is called the *U-partition* of \( V \). The contraction, \( G_U \) say, of \( G \) with respect to the U-partition is called the *Reduced Balance Scheme (RBS)*.

Because of lemma II.1 we have the following result.

**V.3 LEMMA**

\( G_U \) is an open graph with surrounding vertex \( U_0 \). \( G_U \) contains no unmeasured flows.

Assume that, for the original system, the subsystems in \( V_2 \) are ordered such that for all \( k = 0, \ldots, K \) the elements of \( U_k \) have subsequent numbers. Then the definition of the U-partition immediately gives
V.4 Lemma

The matrix $\tilde{M}_{2k}$ has a block diagonal structure where the rows of each diagonal block either correspond to one $U_k$ or to a set of aggregates which are linked by an additional linear relation.

Note that the diagonal blocks mentioned in the lemma are not quadratic in general. An (exactly known) transfer coefficient equation cannot link aggregates since it only affects exactly known and measured flows as well as unmeasured flows of only one aggregate.

The RBS was first introduced by [Vlachek, 1969] and [Mah et al., 1976] in a less stringent graph theoretic fashion. See [Crowe et al., 1983] for a purly algebraic approach in the even more general case where each flow may consist of more than one (chemical) component.

It is clear that each vertex of $G_U = (V_U, E_U)$ either corresponds to a measured subsystem or to an aggregate of a set $U_k$ of unmeasured subsystems in $G$. Accordingly, each balance equation for the RBS is the sum of all balance equations associated with an element of the $U$-partition. Let the balance equations of the RBS be represented by the matrix

$$
(A_{1z}, A_{1z})
$$

(V.12)

Note that (V.12) contains the rows of $(A_{1z} A_{1z})$. The linearly dependent rows in $\tilde{A}_2 = A_2$ are taken care of below. The remaining a priori information contained in the matrix $\tilde{M}$ is incorporated in the following way: we construct a matrix

$$
\tilde{M} = 
\begin{pmatrix}
\tilde{M}_{1z} & \tilde{M}_{1z} & 0 \\
\tilde{M}_{2z} & \tilde{M}_{2z} & \tilde{M}_{2y}
\end{pmatrix}
$$

where the partition into block columns is the same as in (V.4) while the first block row $\tilde{M}_1$ represents the a priori information relevant for the RBS and the second takes up the coefficients of the remaining equations. Thus (V.12) as well as

$$
\begin{pmatrix}
\tilde{T}_{1z,r} & \tilde{T}_{1z,r} \\
\tilde{R}_{1z,r} & \tilde{R}_{1z,r}
\end{pmatrix}
$$

(V.13)

is contained in the first block row of $\tilde{M}$.

Denote by $\tilde{T}_{2,r}$, the $r$-th row of $\tilde{T}_2$, (the procedure for additional linear relations is completely analogous) and assume that $\tilde{M}_2$ already contains the balance equations $A_2$, as well as rows $\tilde{T}_{2,1}$ which have already been added. If $\tilde{T}_{2,y,r}$ is linearly independent of $A_{2y}$ together with the $\tilde{T}_{2,y,k}$ already added, then $\tilde{T}_{2,r}$ is added to $\tilde{M}_2$. Otherwise there is a linear combination of $\tilde{T}_{2,r}$ and the rows of $\tilde{M}_2$, which involves no unmeasured flows. In addition to (V.12) and (V.13), this linear combination is added to $\tilde{M}_1$. (for details see [Gleiß et al., 1998]). Repeat this procedure for all rows of $\tilde{T}_2$.

Assume that linearly dependent rows in $\tilde{M}_2$ as well as rows which represent equations only involving exactly known flows have been deleted. Hence the first block row of $\tilde{M}$ contains all information relevant for the RBS while the second describes the space of admissible unmeasured flows for given measured flows.

V.5 Proposition

Let $S$ be a non-singular row transformation matrix of dimension $(m + \hat{c} + \hat{d}) \times (m + \hat{c} + \hat{d})$. If $S$ describes the procedure for concentrating the information relevant for the RBS in the

---

3Thus the matrix $\tilde{M}$ is not uniquely determined in general. Its right kernel, however, is.
first block row as described above then the north-eastern zero block in

\[
\begin{bmatrix}
\tilde{M} \\
\end{bmatrix} = S \tilde{M} \\
= \begin{bmatrix}
\tilde{M}_{1x} & \tilde{M}_{1z} & 0 \\
\tilde{M}_{2x} & \tilde{M}_{2z} & \tilde{M}_{2y} \\
\end{bmatrix}
\] (V.14)

has a maximal number of rows.

We will call flows which correspond to zero columns of \(\tilde{M}_{1x}\) in (V.14) non-redundant. In the case without transfer coefficient equations and additional linear relations the non-redundant flows are exactly the measured flows between unmeasured subsystems (For the notion of redundant flows cf. [Stanley and Mah, 1981a]). We are now able to give the estimators of the measured flows by means of the RBS:

V.6 Proposition

For positive definite \(\Sigma\) the unique solution of (V.10), (V.11) for the measured flows is given by

\[
\hat{x} = x^* - \Sigma \hat{M}_{1x} (\hat{M}_{1x} \Sigma \hat{M}_{1x})^{-1} (\hat{M}_{1z} x^* + \hat{M}_{1z} z)
\]

which is an efficient estimate of \(x\). The variance-covariance matrix of \(\hat{x}\) is given by

\[
\left( I - \Sigma \hat{M}_{1x} (\hat{M}_{1x} \Sigma \hat{M}_{1x})^{-1} \hat{M}_{1z} \right) \Sigma
\] (V.15)

Non-redundant flows do not influence the reconciliation of the measured flows. For a non-redundant flow \(x_j\) we have \(\hat{x}_j = x^*_j\).

Proof: It is clear that, for positive definite \(\Sigma\), this solution exists, since by construction \(\hat{M}_{1x}\) has full row rank. The uniqueness follows from the fact that the right kernel of a matrix is invariant under row transformations. As has already been mentioned \(\hat{x}\) is efficient since it is a GLS estimator. The variance-covariance matrix is received by direct computation.

The statements on non-redundant flows are consequences of the fact that the columns of \(\hat{M}_{1x}\) are zero columns exactly for non-redundant flows. \(\square\)

Note that the variance of each \(\hat{x}_j\) is smaller than or equal to that of the measurement \(x^*_j\), i.e. the precision of the data has been improved in general.

V.2.2 Estimation of Unmeasured Flows

We still exclude the case of transfer coefficients measured with noise. After estimating \(x\) via the RBS as described above the estimates of the unmeasured flows are determined from

\[
\tilde{M}_{2x} \hat{x} + \tilde{M}_{2z} \hat{x} + \tilde{M}_{2y} \hat{y} = 0
\] (V.16)

so that the unique identifiability of the unmeasured flows depends on the column rank of \(\tilde{M}_{2y}\). However, analogously to lemma V.4, we see that this matrix has a block diagonal structure which allows for a blockwise solution of (V.16). The principal connection between semicycles of unmeasured flows and unidentifiability is discussed in [Crowe et al., 1983], [Mah et al., 1976] and [Stanley and Mah, 1981b].
V.7 Proposition
1. Let \( \hat{y}_{[j]} \) be the subvector of unmeasured flows corresponding to the \( j \)-th diagonal block of \( \bar{M}_2 \). Then \( \hat{y}_{[j]} \) is uniquely determined by (V.16) if and only if for each simple semicycle formed by elements of \( \hat{y}_{[j]} \) a different flow and a different additional linear relation which has not yet been selected for semicycles of another than the \( j \)-th diagonal block, or exactly known transfer coefficient equation can be selected such that this flow is involved in the selected relation.

2. If the \( j \)-th diagonal block fulfills the above condition then \( \hat{y}_{[j]} \) as given by (V.16) is an efficient estimate of \( y_{[j]} \).

Proof: It is clear that an \( l \)-fold semicycle, i.e. a multiple semicycle which contains exactly \( l \) simple semicycles pairwise differing in at least one edge, leads to a column rank defect in \( \bar{A}_2 \) equal to \( l \) (cf. lemma II.7). Thus we need \( l \) equations in addition for which the columns corresponding to \( \hat{y}_{[j]} \) are linearly independent. While transfer coefficient equations cannot involve unmeasured flows corresponding to different diagonal blocks we have to preclude that an additional linear relation is used in more than one diagonal block for resolving a semicycle of unmeasured flows. The second statement is clear since by (V.16) the estimator \( \hat{y}_{[j]} \) is a linear combination of the components of the efficient estimator \( \hat{x} \). □

If there is no a priori information available in the form of (known) transfer coefficient equations or additional linear relations the identifiability condition thus reduces to the absence of semicycles of unmeasured flows. This result is intuitively clear since one could add arbitrary amounts of material to a particular solution for the unmeasured flows in the semicycle which is in accordance with the reconciliated RBS. From these considerations it is straightforward to represent the sets of observationally equivalent transfer coefficients via (V.17).

The variance-covariance matrix for a unique estimator \( \hat{y}_{[j]} \) is easily obtained from (V.15). Furthermore proposition V.7 gives an effective instrument of detecting spots in the system where additional measurements or additional a priori information in the form of transfer coefficient equations or additional linear relations are needed in order to get unique estimates for all flows.

V.2.3 Identification of Subsystems
The subsystems of a material flow system are identified as soon as all elements of the matrix \( M \) are identified, i.e. as soon as all transfer coefficients are uniquely estimated. For the case where noisy measured transfer coefficients are precluded the estimation of transfer coefficients is straightforward though not unproblematic. Because of the assumption (cf. the remark in section V.1) that the transfer coefficient from an inflow of the considered subsystem to the outflow \( f_j \) is the same for all inflows \( f_i \), i.e. \( t_{ji} = t_j \forall i \), we estimate the transfer coefficients as the quotients of the respective flow estimates:

\[
\hat{t}_j = \frac{\hat{f}_j}{\sum_{i:t_i(f_i)\neq 0} \hat{f}_i} \quad (V.17)
\]

Obviously this estimate is not unique if one of the flows involved in (V.17) is not identified uniquely. For exactly known coefficients \( t_j \) we clearly have \( \hat{t}_j = t_j \).

It is important to remark that (V.17) is the maximum likelihood estimator, see [Kendall and Stuart, 1979], p. 137. On the other hand it has an undefined mean and infinite variance in general, since it is the ratio of (dependent) normally distributed variables (cf.
V.2.4 Transfer Coefficients Measured with Noise

If we want to incorporate noisy measurements of transfer coefficients we are confronted with the problem that the restriction (V.6) is non-linear in the variables. One possibility to avoid this problem is a two-step procedure of the following kind:

The first step is equal to the computations described in the previous subsections, i.e. only exactly known a priori information is used for the reconciliation of flows and for the estimation of unmeasured flows and transfer coefficients. In order to get an improved estimate of a transfer coefficient $t_j$ for which also a noisy measurement $t_j^*$ exists, the linear combination (cf. [Bennet, 1963], see also [Finney, 1978], chapters 4 and 14)

$$\hat{t}_j = w\tilde{t}_j + (1-w)t_j^*$$

is computed, where the weight $w$ is given by

$$w = \frac{\hat{\sigma}_j^2}{\hat{\sigma}_j^2 + \hat{\sigma}_j^{*2}}$$

$\hat{\sigma}_j^2$ is an estimator of the variance of the second order Taylor series expansion of $\tilde{t}_j$ around the true value $t_j$, i.e. with $\tilde{f}_{i(i)-k} = \sum \tilde{f}_i f_i$ we get

$$\hat{\sigma}_j^2 = \frac{\sigma_j^2}{(E\tilde{f}_{i(i)-k})^2} + \frac{(E\tilde{f}_j)^2 \text{Var}\tilde{f}_{i(i)-k}}{(E\tilde{f}_{i(i)-k})^4} - 2\frac{E\tilde{f}_j \text{Cov}(\tilde{f}_{i(i)-k}, \tilde{f}_j)}{(E\tilde{f}_{i(i)-k})^3}$$

where in addition the expected flow values are replaced by the corresponding estimates.

For the second step it is assumed that the improved estimates $\hat{t}_j$ are exactly known transfer coefficient values. Thus we may add new transfer coefficient equations to the a priori information as described above proposition V.5 and repeat the reconciliation and estimation procedure for exactly known a priori information.

Obviously, the flow variance estimates as given in (V.15) are no longer valid, neither is the efficiency of the flow estimates themselves. Another practical short-coming of this two-step approach arises if all inflows of a subsystem are exactly known while one of its outflows as well as the transfer coefficient associated with this outflow are measured with noise. In this case the outflow estimate given by the second step is assigned a zero variance which is certainly wrong. For an alternative procedure see [Gleiß et al., 1998].

Finally, we have to consider a special case:

**Definition:** A measured transfer coefficient which is contained in a transfer coefficient equation which decreases the degree of freedom for the computation of the estimates of the unmeasured flows, is called a non-redundant transfer coefficient.

Note that the information contained in the measurement variance of a non-redundant transfer coefficient is not exploited. In this case we act as if $t_j^* = t_j$ holds.
V.3 Origins Analysis

For practical reasons it is interesting to know more about the internal (directed) dependen-
cies between different flows of the system under consideration. The aim of origins analysis,
as originally proposed by [Van der Voet et al., 1995a], is to find sets of imports and internal
flows which give a complete physical explanation of a considered flow and which do not in-
fluence each other (in the physical sense, i.e. there is no path containing any two of them).
The analysis is based on the structure of the estimated system. In this way, one gets a clear
quantitative picture of which flows contribute to a given flow to what extent.

**DEFINITION:** A *contributor set* is a maximal subset \( C \) of the set of all internal and import
flows such that the elements of \( C \) do not influence each other. For a given flow \( f_j \) each
element of a *contributor set for* \( f_j \), denoted by \( C(f_j) \), in addition influences \( f_j \).

Note that for a given flow \( f_j \) different contributor sets may have a non-empty intersection.
The above definition implies that flows (edges) which are part of a cycle cannot be elements
of a contributor set since such flows influence themselves. Thus it suffices to investigate the
graph \( \mathcal{G}^- = (V^-, E^-) \) which emerges from the system graph as follows: First remove the
exports and contract all cycles and then add the surrounding vertex explicitly to the graph
so that the imports of \( \mathcal{G} \) are now internal flows of \( \mathcal{G}^- \). Let the number of vertices in this
graph be denoted by \( m^- \). Clearly, \( \mathcal{G}^- \) is not an open graph. Its shape could be called a
"semitree", since it contains no cycles but may well contain semicycles. This means that
branches of this tree may "grow together" (in accordance with the "growing direction"). As a
consequence we get the following graph theoretic characterisation of a contributor set which
will be the basis of the construction algorithm presented below.

V.8 **Proposition**

An edge set \( C \subset E \) is a contributor set if and only if the corresponding edges on \( \mathcal{G}^- \) form a
maximal edge-disjoint union of positive cutsets \( C_i \) on \( \mathcal{G}^- \) such that

\[
V^{-i}_1 \cap V^{-j}_2 = \emptyset \quad \forall i \neq j
\]  

(V.18)

holds, where \( (V^{-i}_1, V^{-j}_2) \) is the partition of \( V^- \) associated with the positive cutset \( C_i \).

In the proof of the following result we give a construction algorithm for contributor sets.

V.9 **Proposition**

There are \( m^- \) linearly independent positive cutsets on \( \mathcal{G} \).

**Proof:** Consider the graph \( \mathcal{G}^- \). Since it contains no cycles there exists a vertex, \( i_1 \) say,
without outflows. Thus the incidence cut corresponding to \( i_1 \) is the first positive cutset \( C_1 \).
Because of the same reason we can now find a vertex \( i_2 \) such that the vertex corresponding
to \( \{i_1, i_2\} \) in the contraction with respect to

\[
\{\{i_1, i_2\}\} \cup \{\{i\}, i \in V^- \setminus \{i_1, i_2\}\}
\]

has no outflows. This gives the second positive cutset as the incidence cut of this aggregate
which is the sum of the incidence cuts of \( i_1 \) and \( i_2 \) in \( \mathcal{G} \). Note that \( C_1 \) and \( C_2 \) correspond
to linearly independent rows in the cut matrix of \( \mathcal{G} \), since the underlying incidence cuts
(corresponding to \( i_1 \) and \( i_2 \) do so). This procedure can be repeated until all \( m^- \) vertices of
\( \mathcal{G}^- \) are used up. If, for the first time, at the \( k \)-th step in this algorithm there are more than
one choices for the next vertex, \(i_{k,1}, \ldots, i_{k,L}\) say, then proceed, for each \(l = 1, \ldots, L\), with the vertex corresponding to \(\{i_1, \ldots, i_{k-1}, i_k, l\}\) in the contraction with respect to

\[
\{\{i_1, \ldots, i_{k-1}, i_k\} \cup \{i\}, i \in V^\sim \setminus \{i_1, \ldots, i_{k-1}, i_k\}\}
\]

\[\square\]

It remains to compute, for a chosen contributor set \(C(f_j)\), the percentage of contribution of each element \(f_i\) of \(C(f_j)\). While the estimated transfer coefficients give such information in the case where \(t(f_i) = s(f_j)\) holds, we need here to consider the influence of \(f_i\) onto \(f_j\) via all paths of all possible lengths.

For this purpose let the matrix \(D\) with elements \(d_{ij}\) \((i, j = 1, \ldots, n)\) be constructed as follows: there is a non-zero entry at the \((i, j)\)-position, which is equal to \(\hat{t}_{ij}\), if and only if \(t(f_i) = s(f_j)\) and \(f_i, f_j \neq 0\) hold. Thus the \((i, j)\)-element of \(D^\delta\), for a positive integer \(\delta\), gives the influence of \(f_i\) onto \(f_j\) via all paths of length \(\delta\). Finally, we may compute the matrix

\[
\sum_{\delta > 0} D^\delta
\]  

(V.19)

This sum is finite if and only if there are no cycles in the system graph. In the case where the considered system contains no traps it is easy to see (cf. theorem VI.4) that (V.19) converges to

\[
\hat{D} = (I - D)^{-1}
\]

so that the elements of \(\hat{D}\) consider all paths of all possible lengths. The percentage of contribution of flow \(f_i\) to flow \(f_j\) for \(f_j \neq 0\) is calculated as

\[
\frac{\hat{d}_{ij} \hat{f}_i}{\hat{f}_j} \cdot 100\%
\]

For a contributor set these percentages sum up to 100%. It is important to note that, in general, the percentage of contribution is not identical to the effect, which a modification of the value of \(f_i\) has on the value of \(f_j\). The reason is that for answering such system theoretic questions also upstream dependencies and additional linear relations have to be taken into account. In [Gleiß et al., 1998] a way to calculate such effects is presented. Based on this control analysis simulations can be performed.

Remark: It is easy to apply what could be called a destination analysis. This kind of analysis yields sets of internal and export flows into which a considered flow is divided up and which are not influenced by each other. In order to do so an origins analysis has to be performed on the system where all flow directions have been reverted. \(<\)

V.4 Error Propagation

In this section we want to investigate according to which graph theoretic rules the measurement variances contribute to the variances of the flow estimates by disentangling (V.15). It is, however, important to observe that properties like: The variance of \(\hat{x}_j\) is more sensitive to the measurement variance of flow \(i\) than to that of flow \(k\), are not of a generic type. Another issue in the context of measurement variances, which also leads to complex graph theoretic problems, deals with gross errors, i.e. systematic errors which occur due to
an incomplete or inaccurate system representation. This topic is not treated in this work, see [Crowe, 1988], [Mah et al., 1976] and [Romagnoli and Stephanopoulos, 1981].

The results presented in this section are restricted to the case with diagonal $\Sigma$ and without transfer coefficient equations and additional linear relations. In addition we refer to the reduced balance scheme (see subsection V.2.1), i.e. it is assumed that no unmeasured flows are present. For simplicity let us also assume that there are no exactly known flows\footnote{Otherwise consider the graph where all exactly known flows and all subsystems which are incident only with exactly known flows are deleted.}. Thus we have $f = x$ and $M = M = A = A_1_2$ if not stated otherwise.

Let us define the following variables

\[
\begin{align*}
S &= \sum_{J' \in J} \prod_{i \in J'} \sigma_i^2 \\
S_i &= \sum_{J' \in J_i} \prod_{i \in J'} \sigma_i^2 \\
S_{ij} &= \sum_{J' \in J_i \cap J_j} \prod_{i \in J'} \sigma_i^2
\end{align*}
\] (V.20)

where $J$ denotes the set of all index sets of edges which give a spanning tree of the system graph and where $J_i$ and $J_{ij}$ denote the set of all index sets of edges which do not contain the index $i$ (and the index $j$, respectively) and which, together with the $i$-th edge (and the $j$-th edge, respectively), give a spanning tree of the system graph. Thus we have

$$J' \in J_i \Leftrightarrow i \not\in J' \cap J' \cup \{i\} \in J$$

An interpretation of the definitions (V.20) can be given as follows: weight each edge of the system graph by the variance of the associated measurement. Then $S$ is the sum of the weights of all spanning trees, while $S_i$ and $S_{ij}$ are the sum of the weights of all spanning trees containing the $i$-th (and the $j$-th, respectively) flow.

Let $A_p$ denote the matrix which is created from $A$ by eliminating the $p$-th row, i.e. $A_p$ is the incidence matrix of the contraction of $G$ with respect to

$$\{\{0, p\} \cup \{i\}, i \in V \setminus \{p\}\}$$

V.10 **Lemma**

1. Using the definitions above we have

$$\det(\Sigma A'_i) = S$$

2. Define $J'^p$ as the set of all index sets of edges which give a spanning tree of the system graph after deleting vertex $p$ as well as after deleting vertex $q$. Then we have

$$\det(A_p \Sigma A'_q) = (-1)^{p-q} \sum_{J' \in J'^p} \prod_{i \in J'} \sigma_i^2$$

**Proof:** Both statements are consequences of the Binet-Cauchy-formula (see, e.g., [Lancaster and Tismenetsky, 1985]) when the special structure of $A$ and the diagonality of $\Sigma$ is taken into account.

1. By the Binet-Cauchy-formula for the second equality below we have, with $A(J')$ denoting the matrix consisting of the columns given by the index set $J'$,

$$\det(\Sigma A') = \det((\Sigma A') A') = \sum_{J' \in J} \det((\Sigma A_{\{J'\}} A'_{\{J'\}})) = \sum_{J' \in J} \left( \prod_{i \in J'} \sigma_i^2 \right) \det(A_{\{J'\}} A'_{\{J'\}}.$$
Note that for diagonal $\Sigma$ the equality $(A\Sigma)(J') = A_{(J')}\Sigma_{(J')(J')} \equiv$ holds, where $\Sigma_{(J')(J')}$ selects the columns and rows of $\Sigma$ according to $J'$. By lemma II.7 a spanning tree of the system graph (including the surroundings) gives a regular choice of columns in $A$. $A_{(J')}$ can be triangularised by an appropriate reordering of the rows and columns, so that $\det(A_{(J')}) = \pm 1$.

2. Similarly as before we have

$$\det(A_p, \Sigma A_q) = \sum_{J' \in J^p} \left( \prod_{i \in J'} \sigma_i^2 \right) \det(A_{p,(J')}) \det(A_{q,(J')}).$$

It remains to show that for given $J' \in J^q$ the product of the two determinants equals $(-1)^{q-p}$. First note that since $J'$ is a regular choice of columns for both $A_p$ and $A_q$ there cannot be any connection in $A_{(J')}$ between subsystem $p$ or $q$ and the surroundings; otherwise either $A_{p,(J')}$ or $A_{q,(J')}$ would have a zero column. Thus adding an $m$-th column corresponding to a flow from $q$ to $p$ to the $m \times (m - 1)$ matrix $A_{(J')}$ gives a semicyclic, i.e. a singular matrix. Expanding the resulting matrix along the added column therefore gives

$$1 \cdot (-1)^{m+p} \det(A_{p,(J')}) + (-1) \cdot (-1)^{m+q} \det(A_{q,(J')}) = 0$$

which yields

$$\det(A_{p,(J')}) \det(A_{q,(J')}) = (-1)^{q-p}(\det(A_{q,(J')}))^{-2}$$

The statement is now proved because $\det(A_{q,(J')}) = \pm 1$ since the columns corresponding to $J'$ give a spanning tree of the system graph without subsystem $q$ (note that by what was said above cutting off subsystem $q$ gives in $J'$ at least one connection to the surroundings of the reduced graph). □

Recall that by proposition V.6 the variance-covariance matrix of the flow estimates is given by

$$\text{Var} \hat{x} = \Sigma - \Sigma A' (A \Sigma A')^{-1} A \Sigma \quad \text{(V.21)}$$

V.11 PROPOSITION

Using the definitions (V.20) we have

$$\text{Var} \hat{x}_j = \sigma_j^2 \left( 1 - \frac{S_j}{S} \right) \leq \sigma_j^2$$

Proof: First of all the (trivial) inequality follows from $J_j \subseteq J$. With $\bar{a}_j$ denoting the $j$-th column of matrix $A$ we have from (V.21) and from the diagonal of $\Sigma$

$$\text{Var} \hat{x}_j = \sigma_j^2 - \sigma_j^2 \bar{a}_j(A \Sigma A')^{-1} \bar{a}_j$$

$$= \sigma_j^2 - \frac{\sigma_j^2}{\det(A \Sigma A')} \bar{a}_j K' \bar{a}_j,$$

where $K = (A \Sigma A')$ denotes the cofactor matrix of $(A \Sigma A')$.

Thus it remains to show that

$$\sigma_j^2 \bar{a}_j K' \bar{a}_j = S_j$$

With $K_{pq}$ denoting the $(p,q)$-element of $K$ $(p,q = 1, \ldots, m)$ so that

$$K_{pq} = (-1)^{p+q} \det(A_p, \Sigma A_q)$$
and s and t denoting the starting and the terminal subsystem of flow j, respectively, we have

$$\bar{u}^j K \bar{u}^j = K_{tt} + K_{ss} - K_{st} - K_{ts}. \quad (V.22)$$

If flow j is an input or an output flow into the whole system, the right hand side of (V.22) reduces to \(K_{tt}\) or \(K_{ss}\), respectively, and the following considerations work accordingly.

According to the second part of lemma V.10 the following equations hold:

$$K_{tt} = \sum_{j' \in J'' \cap J'} \prod_{i \in j'} \sigma_i^2,$$

$$K_{ss} = \sum_{j' \in J'' \cap J'} \prod_{i \in j'} \sigma_i^2,$$

where \(J'' (J'^{ss})\) is the set of all index sets of edges which give a spanning tree of the system graph after deleting the vertex \(t\) (the vertex \(s\)), i.e. each \(J'\) corresponds to a regular choice of columns of \(A_s\) (of \(A_s\)).

Furthermore we have

$$K_{ts} = \sum_{j' \in J'^{ss} \cap J'} \prod_{i \in j'} \sigma_i^2 = K_{ts}$$

By definition \(J'^{ss} = J'^{st} = J'^{ss} \cap J''\) and thus

$$\left((J'^{ss} \setminus J'^{st}) \cup (J'^{st} \setminus J'^{ss})\right) = J'^{ss} \oplus J'^{st},$$

where \(\oplus\) denotes the symmetric difference. Together with equation (V.22) this implies

$$\bar{u}^j K \bar{u}^j = \sum_{j' \in J'^{ss} \oplus J''} \prod_{i \in j'} \sigma_i^2$$

The proof is thus completed by showing that \(J_j = J'^{ss} \oplus J'^{st}\). Note that, for \(J'\) being a choice of \(m-1\) flows, \(J' \cup \{j\}\) gives a cycle if and only if \(J' \in J'^{st}\) holds.

For \(J' \in J'^{ss} \oplus J'^{st}\) we have \(J' \cup \{j\} \in J\) since, first, the added (s-th or t-th) subsystem is covered by flow \(j\) and, secondly, no cycle is built by adding this flow, since otherwise \(J' \in J'^{st}\), which is a contradiction. Hence \(J' \supset J'^{ss} \oplus J'^{st}\).

Assume on the other hand that there exists a \(J' \in J_j\) with \(J' \not\in J'^{ss} \oplus J'^{st}\). Then either \(J' \in J'^{ss} \cap J'^{st} = J'^{st}\) or \(J'\) is in the complement of \(J'^{ss} \cup J'^{st}\). The first case implies that \(J' \cup \{j\}\) gives a cycle, so that \(J' \cup \{j\} \not\in J\), which is a contradiction. From the second case it follows that the choice of flows \(J'\) does not cover all subsystems excluding \(s\) and \(t\); this again is a contradiction since then \(J' \cup \{j\}\) gives a tree which is not a spanning tree. \(\square\)

If we consider a general system graph, i.e. we drop the assumptions made in the beginning of the section, we can draw the following conclusions.

V.12 Corollary

1. \(\text{Var } \hat{x}_j = \sigma_j^2\) holds if and only if flow \(j\) is non-redundant.

2. \(\text{Var } \hat{x}_j = 0\) holds if and only if beside flow \(j\) only measured flows which lead into a trap, or exactly known flows are incident at the same subsystem.
Proof: For the first statement note that the flow \( j \) is non-redundant if and only if the \( j \)-th column of \( A \) contains only zeroes, so that this flow is part of no spanning tree of the reduced balance scheme, i.e. \( S_j = 0 \). The second statement follows from the fact that by the proposition a zero variance of the \( j \)-th flow is equivalent to \( S_j = S \) which means that this flow is contained in every spanning tree. It is then easy to observe that this is equivalent to the cases enlisted in the corollary. □

Let us define \( S_{(j)} = S - S_j \), \( S_{(i,j)} = S_i - S_{ij} \), and analogously for \( S_{(i,j)} \) and \( S_{(i,j)} = S_{ij} - S_{(ij)} \). It is then easy to calculate the derivatives of the variance of an estimated flow with respect to the measurement variance of another flow.

V.13 Proposition
Using the above definitions we have

\[
\frac{\partial \text{Var} \hat{x}_j}{\partial \sigma_j^2} = \left( 1 - \frac{S_j}{S} \right)^2
\]

and for \( i \neq j \)

\[
\frac{\partial \text{Var} \hat{x}_j}{\partial \sigma_i^2} = \frac{\sigma_j^2}{\sigma_i^2} \left[ S_{(i,j)} S_{(i)} - S_{ij} S_{(i,j)} \right]
\]

(V.23)

Proof: Note that the derivatives of the expressions in (V.20) obey the following rules:

\[
\frac{\partial S}{\partial \sigma_i^2} = \frac{S_i}{\sigma_i^2}, \quad \frac{\partial S_j}{\partial \sigma_i^2} = \frac{S_{ij}}{\sigma_i^2}, \quad \frac{\partial S_j}{\partial \sigma_j^2} = \frac{S_j}{\sigma_j^2}
\]

We therefore get

\[
\frac{\partial \text{Var} \hat{x}_j}{\partial \sigma_i^2} = -\frac{\sigma_j^2}{S^2} \left[ S_{(i,j)} S - S_{ij} S_i \right]
\]

By subtracting \( S_{ij} S_j \) from both terms in the first equality and \( S_{(i,j)} S_{ij} \) in the second equality of

\[
S_{ij} S - S_i S_j = S_{ij} S_{(i)} - S_{(i,j)} S_j = S_{ij} S_{(i,j)} - S_{(i,j)} S_{(i)}
\]

the second result is proved. The first result is received by direct computation. □

Note that the index sets underlying the expression in square brackets of (V.23), namely \( J_{(i,j)}, J_{(i,j)}, J_{ij} \) and \( J_{(i,j)} \), using an obvious notation, are disjoint. They give a partition of the set of all spanning trees on \( G \). Since furthermore the same expression is symmetric with respect to \( i \) and \( j \) we get the following

V.14 Corollary
For \( i \neq j \)

\[
\frac{\sigma_j^2}{\sigma_i^2} \frac{\partial \text{Var} \hat{x}_j}{\partial \sigma_i^2} = \frac{\sigma_j^2}{\sigma_j^2} \frac{\partial \text{Var} \hat{x}_i}{\partial \sigma_j^2}
\]

holds.
CHAPTER VI

A DYNAMIC MODEL WITH EXACT LIFETIME

In Material Flow Analysis dynamics come in via stocks, where a portion of the substance under consideration enters a subsystem and does not leave it within the same balancing period. By the lifetime of a stock we mean the residence time of the material in the stock. In general, the lifetime follows some distribution on the non-negative integers, which, for instance, corresponds to the disposal behaviour in the case of materials within (durable) consumer goods or to geo-physical depletion laws in the case of environmental stocks.

A subsystem of a dynamic material flow system has the inner structure shown in fig. VI.1, where balance equations hold for the inner static subsystems. The transfer function for the \( j \)-th subsystem in general is given by

\[
 k_j(s) = \sum_{t \geq 0} w_l(p_j)s^{-t}
\]

where the weighting matrices \( w_l \) describe a stock behavior depending on a stock parameter \( p_j \). Here the law of the conservation of mass implies that the column sums of the \( w_l \) sum up to a value less than or equal to one.

The simplest kind of such a pattern, called exact lifetime pattern, is the case when the outflow during period \( t \) is equal to the inflow during period \( t - \tau \), i.e.

\[
 w_l(\tau_j) = \begin{cases} 
 1 & \text{for } l = \tau_j \\
 0 & \text{else}
\end{cases}
\]

The lifetimes of all subsystems might be known a priori or be part of the set of parameters to be estimated from measurement data.

In this chapter we will present results in the context of identification of systems with exact lifetimes. In the two succeeding chapters we will see that more complicated patterns of stock dynamics can - at least in the case of some further restrictions - be traced back to this simple prototype. In the following we will list and discuss a catalogue of assumptions which are used to formulate the model classes for the different lifetime patterns.
Figure VI.1: The transfer coefficients of the dynamic subsystem are the (static) transfer coefficients $t_1$ and $t_2$ of the right-hand static subsystem.

### VI.1 General Assumptions

The first set of assumptions concerns the system graph, i.e., the weighted graph which directly corresponds to the flow sheet (see chapter III) describing the material flow system under consideration. The system graph will always be denoted by $G = (V, E)$.

**Assumption 1**

- a: The system graph is a connected open graph.
- b: There are no parallel edges on the system graph.
- c: There are no loops on the system graph.

As has already been discussed in chapter III it is useful to restrict the investigations to open systems, i.e., where there is some kind of surrounding with which the considered system exchanges material. Although there is no technical reason for doing so, we will assume that the system graph is connected since otherwise we might as well consider each component separately. Loops, which, from a practical point of view, are not useful in the case of exact lifetimes, will only be used in order to describe a certain kind of stock behaviour in chapter VIII. Note that 1b also precludes more than one import or export per subsystem.

**Assumption 2**

- a: Each outflow of a dynamic subsystem only depends on the sum of the respective inflows.
- b: There are no static subsystems, i.e., all lifetimes are greater than zero.
- c: For each subsystem the transfer coefficients corresponding to the set of its outflows sum up to one.

Since it is reasonable to assume that all flows which enter the same stock have the same stock behaviour, we also postulate in 2a that their partitioning between the outflows of the corresponding subsystem is the same for all of them. Hence only one transfer coefficient is associated with each flow in the system. Note that this assumption allows us to work with
a weighted graph, since then the weight of an edge is identical with the transfer coefficient of the respective flow. It is important to note that the static subsystems within a dynamic system may have practical relevance. The assumption 2c, which is based on the law of mass conservation and which gives the balance equations, will only be dropped for some intermediate results. Note that under 2c there are less free parameters than transfer coefficients and that, for material flow systems, this assumption is part of the a priori knowledge which is not contained in the flow sheet.

The next set of assumptions refers to the measurement model. While the first condition is quite natural and the second seems to hold in most case studies, the others obviously restrict the practical applicability of the model.

**Assumption 3**

a: At least one internal or export flow is observed.

b: Stocks are not observed (directly).

c: A flow is measured or unmeasured in all periods of observation.

d: The system theoretic inputs are identical with the imports all of which are observed.

Single assumptions will be referred to as assumption 1b, for example. We will often refer to a whole set of assumptions as assumptions 1. Additional, more specific assumptions will be formulated in the model class sections of this and the succeeding chapters.

## VI.2 Generic Properties

**Definition:** A subset \( V \) of \( \mathbb{R}^r \) is called **algebraic** if there is a set of polynomials \( g_j \in \mathbb{R}[x_1, \ldots, x_r] \), \( j = 1, \ldots, l \) with

\[
V = \{ d \in \mathbb{R}^r : g_1(d) = 0, \ldots, g_l(d) = 0 \}.
\]

An algebraic set \( V \) is called **proper** if it is a strict subset of \( \mathbb{R}^r \).

Of course, this definition may be transferred to subsets of other base sets than \( \mathbb{R}^r \). In our case we will in particular consider subsets of a set \( N \subseteq \mathbb{R}^r \) so that (VI.1) has to be replaced by \( V = \{ d \in N : \ldots \} \).

**Definition:** A property that may be assigned to a matrix \( M \) with \( r \) non-zero elements holds **generically** in \( N \) if there exists a proper algebraic set \( V \subseteq N \) such that the property holds for all elements of \( N \) except those in \( V \).

Note that such a property is often said to hold **structurally**, see e.g. [Reinschke, 1988], where the term **generic** is used for what we will define as \( \theta \)-generic. In [Murota, 1987] the **term-rank** denotes the generic rank while what is called **generic rank** there is the \( \theta \)-generic rank in our notation. In econometrics the term **structural** assigned to a property such as identifiability marks the case where the considered property is looked at under restrictions on the elements of the system matrices, cf. [Hannan and Deistler, 1988]. Since this is always the case in the context of compartmental models the definitions of reachability, identifiability etc. will implicitly denote structural reachability, structural identifiability etc. in the sense just mentioned.
A Dynamic Model with Exact Lifetime

VI.3 Model Class

We use a (discrete-time) state space model for the material flow system:

\[
\begin{align*}
x_{t+1} &= Ax_t + Bu_t \\
y_t &= Cx_t + Du_t
\end{align*}
\]

Here the vector \( u_t \) denotes the imports into the whole system, the vector \( y_t \) consists of the observed internal and export flows and the state vector \( x_t \) comprises all stock levels of the dynamic subsystems. Thus here the state dimension is given a priori.

The involved matrices are said to be the system matrices, the matrices \( A, B \) and \( C \) in particular are called the state transformation matrix, the input matrix and the observation matrix, respectively.

By a system structure \([A, B, C]\) (called "fixed structure system" in [Cobelli et al., 1979a]) we understand the model class defined by a classification of the elements of the system matrices \( A, B \) and \( C \) into zero and (independently varying) non-zero elements. For \( \theta \)-generic considerations also the parameterisation \( \theta \) is part of the definition of the system structure \([A, B, C, \theta]\).

A numerical realisation of \([A, B, C]\), i.e. a matrix triple \((A_0, B_0, C_0)\) which has zero elements in accordance with the considered system structure, is denoted by \([A, B, C]_{d_0}\) if the non-zero elements are exactly the elements of \( d_0 \in N \) (in a given order). For a numerical realisation of \([A, B, C, \theta]\), denoted by \([A, B, C, \theta]_{d_0}\), the vector \( d_0 \) in addition has to fulfill the restrictions given by \( \theta \), i.e. \( d_0 \in \theta(P) \).

A vector \( d_0 \in N \) will be called, e.g., reachable if \([A, B]_{d_0}\) is reachable in the usual sense, provided that the underlying system structure is clear from the context.
Figure VI.2: A subsystem with given exact lifetime $\tau$ as a chain of $\tau$ subsystems with lifetime one.

In the case of exact lifetimes we often assume (for simplicity and - in most cases - without loss of generality) that all lifetimes are equal to one, since a subsystem of lifetime $\tau > 1$ can easily be modeled as a chain of $\tau$ subsystems each of which has lifetime one, see fig. VI.2.

In this case the extended system graph $\tilde{G}$ is the graph where each subsystem is replaced by such a chain of appropriate length. Accordingly, the system matrices corresponding to this extended graph are denoted by $\tilde{A}, \tilde{B}, \tilde{C}$ and $\tilde{D}$.

Let us define a static path as a path all vertices of which correspond to static subsystems except possibly the first and the last one. In particular a static path of length one is an edge and a static path of length zero describes the special case where the source and the terminal vertex of the path coincide. Because of the assumptions 1 and 3 the system matrices thus have the following structure according to the graph $\tilde{G}$. There is a non-zero element in $\tilde{A}$ at the $(i,j)$-position if and only if there is a static path in $\tilde{G}$ from $j$ to $i$. The matrix $\tilde{B}$ has a non-zero element at the $(i,l)$-position if and only if the $k$-th import enters subsystem $i$ or if it enters a static subsystem from which there is a static path leading to $i$. There is a non-zero entry at the $(k,j)$-position of $\tilde{C}$ if and only if the $k$-th observed flow is an outflow of subsystem $j$ or if it is an outflow of a static subsystem which is reached from $j$ by a static path. If, in addition, we assume 2b then $\tilde{D}$ is a zero matrix of appropriate dimension and all static paths mentioned above are of length one or zero, respectively. In any case, each non-zero element contains the portion which, along the respective static path, flows from an input or a stock to an output or to another stock, respectively. It follows that, in the following definition, $N = [0,1]^r$ holds where $r$ is the number of non-zero elements in $\tilde{A}, \tilde{B}, \tilde{C}, \tilde{D}$.

The state transformation matrix for general lifetimes $\tau_j, j = 1, \ldots, m$ has the following form: the diagonal block corresponding to the subsystem $j$ in $\tilde{G}$ equals

$$
\begin{pmatrix}
0 \\
\vdots \\
I_{\tau_j - 1} \\
0 & \ldots & 0
\end{pmatrix}
$$

where $I_k$ is the $k$-dimensional identity matrix. For $i \neq j$ the $(i,j)$-block in $\tilde{A}$ is the $\tau_i \times \tau_j$ matrix the only non-zero element of which is the appropriate transfer coefficient in the south-western corner.

For the description of the dynamic model with exact lifetimes we also assume 2b and 2c. By the balance equations, the set of free parameters, $P_1$, is given as follows: For each subsystem $k$ the (non-negative) transfer coefficients associated with its outflows can be described by $n^+(k) - 1$ (non-negative) free parameters ($n^+(k)$ denotes the number of successors of $k$) the sum of which has to be less than one. This gives $P_1$ as the cartesian product of the appropriate unit simplices:

$$P_1 = S_{n^+(1)-1} \times S_{n^+(2)-1} \times \ldots \times S_{n^+(m)-1}$$
where $\mathcal{S}_1$ is the (closed) convex hull of the zero vector and the unit vectors in $\mathbb{R}^d$. The dimension of $P_1$ is thus given by

$$\sum_{k=1}^{m} (n^+(k) - 1)$$

which is equal to $n - n^m - m$ where $n^+(k)$ denotes the number of outflows of the $k$-th subsystem and $n^m$ denotes the number of inputs (of the whole system).

For the deduction of the identifiability conditions we need the parameterisation $\bar{\theta}_1 : \bar{P}_1 \to N$ which attaches to each non-zero element in the system matrixes the weight of the corresponding edge on the system graph. Thus the non-zero elements of $[A, \bar{\theta}_1]$ contain the corresponding transfer coefficients$^1$. This means that only the restrictions on the input and on the observation matrix are taken into account in addition to the trivial parameterisation, so that all non-zero elements of $[A, \bar{\theta}_1]$ are free (non-negative) parameters but the non-zero entries of $[B, \bar{\theta}_1]$ are equal to one and an entry of $[C, \bar{\theta}_1]$ is identical to an entry in the same column of $[A, \bar{\theta}_1]$ if it does not correspond to an export. Thus $\bar{P}_1$ can be described similarly to (VI.13) where each factor of the cartesian product, however, is given by $R_{n^+(k)}$.

Let $\theta_1 : P_1 \to N$ denote the parameterisation which, in comparison to $\bar{\theta}_1$ do take the balance equations into consideration.

Hence under 2b the system graph is identical with the Coates graph associated with $[A, \bar{\theta}_1]$ after imports have been added according to the matrix $[B, \bar{\theta}_1]$, the columns of which now are unit vectors, and exports according to whether the respective column sum of $[A, \bar{\theta}_1]$ is either strictly less than or equal to one ($\bar{\theta}_1$-generically). The entries of the state transformation matrix are the respective transfer coefficients. Since we observe outflows of the stocks in the system, also the observation matrix contains transfer coefficients which are, in the case where the observed flow is not an export, identical with those in $[A, \bar{\theta}_1]$.

Note that, independently of 2b, the state transformation matrix is a compartmental matrix. For technical reasons we will also need the following condition:

**Assumption 4**

There are no cycles on $\mathcal{G}$ differing in at least one edge which have the same length (counted as the sum of the lifetimes of the involved subsystems). For each pair $(i,j)$ of an input $e_i$ and an output $e_j$ there are no paths from $t(e_i)$ to $s(e_j)$ differing in at least one edge which have the same length.

Note that this assumption implies that there is at most one loop on the system graph. Summing up, the parameterisation $\theta_1$ implicitly assumes all conditions 1, 2 and 3, while $\bar{\theta}_1$ assumes only 1, 2a, 2b and 3.

### VI.4 Stability

In this section we assume that the lifetimes are a priori known for all subsystems.

**Definition:** A state space system with state transformation matrix $A$ is called *asymptotically stable* if the eigenvalues of $A$ lie in the open unit disc.

---

$^1$This sloppy formulation means that $\bar{\theta}_1$ maps to each non-zero element of $A$ a (different) free parameter $\bar{\theta}_1 \in P_1$, which corresponds to the respective transfer coefficient.
VI.4 Stability

We will also say that the matrix $A$ is asymptotically stable if the above condition is satisfied. The following lemmas will not be proved here. The first one follows from the Perron-Frobenius theorem, the second lemma is a corollary of the theorem of Geršgorin and of the theorem of Taussky, see, e.g., [Lancaster and Tismenetsky, 1985].

VI.1 Lemma
Let $A \in \mathbb{R}^{m \times m}$ have non-negative elements. Then $A$ has a real eigenvalue equal to its spectral radius.

VI.2 Lemma
Let $A \in \mathbb{R}^{m \times m}$ be irreducible with non-negative elements. If all column sums in $A$ are less than or equal to one, i.e., if $\mathbf{1}^\top A \leq \mathbf{1}$ holds, and if the inequality is strict for at least one column then the spectral radius is strictly less than one.

VI.3 Corollary
For an irreducible compartmental matrix $\mathbf{1}^\top A = \mathbf{1}$ is equivalent to the existence of an eigenvalue of $A$ which is equal to one.

Let us now consider a system structure $[A, \theta_1]$. It is clear that a vertex $j$ has an export if and only if it holds $\theta_1$-generically that the $j$-th column sum is strictly less than one. Therefore a strong component is a trap (note that a trap always has to be a strong component) if and only if the column sums in the corresponding diagonal block in (II.6) are all equal to one $\theta_1$-generically. For the special case when $[A]$ is irreducible the whole system is a trap if and only if all column sums in $A$ are $\theta_1$-generically equal to one.

Although the following theorem can be found in, e.g., [Van Den Hof, 1998], a proof will be outlined here, since the applicability of the theorem to the various cases of system dynamics has to be shown later on.

VI.4 Theorem
The system structure $[A, \theta_1]$ is $\theta_1$-asymptotically stable if and only if $\mathcal{G}$ contains no traps.

Proof: The following proof is established for a numerical realisation $A$ of the given system structure. Adding "$\theta_1$-generically" to all specific statements gives the proof of the theorem. Furthermore it is clear that there are no traps in $\mathcal{G}$ exactly if there are no traps in $\mathcal{G}$.

First we show that instability occurs if and only if $A$ has an eigenvalue equal to one. The sufficiency part is clear from the definition of stability. For the necessity part we assert that all eigenvalues lie on the closed unit disk. This is true because for a compartmental matrix $A$ with elements $a_{ij}$ all Geršgorin circles ($j = 1, \ldots, m$)

$$\left\{ z : |z - a_{jj}| \leq \sum_{i \neq j} |a_{ij}| \right\}$$

are contained in the closed unit disk. Applying lemma VI.1 to matrix $A$ shows that instability implies an eigenvalue equal to one.

Now we have to show that an eigenvalue equal to one is necessary and sufficient for the existence of a trap, i.e., for reducible $A$, of a diagonal block $B_{ii}$ in (II.6) with $\mathbf{1}' B_{ii} = \mathbf{1}'$.

The case where $A$ is irreducible is covered by corollary VI.3.

Suppose there exists such a block $B_{ii}$, so that $B_{ii}$ has an eigenvalue equal to one. Then it is clear from the block triangular form of $\mathbf{P}' A \mathbf{P}$ that also $A$ has an eigenvalue equal to one. On the other hand suppose that one is an eigenvalue of $A$. Thus there exists a vector $v \neq 0$ such that $\mathbf{v}' (\mathbf{P}' A \mathbf{P}) = \mathbf{v}'$. The first block of this equation gives $\mathbf{v}' B_{11} = \mathbf{v}'$. By lemma II.9 the submatrix $B_{11}$ is either irreducible, so that by lemma VI.2 we have $v_1 = 1$ terminating
the proof, or equal to zero, in which case it follows that \( v_1 = 0 \). Since then the second block equation is \( v_2 B_{22} = v_2 \) we can proceed as before. The search for a block \( B_{ij} \) with all column sums equal to one must succeed since otherwise \( (P'AP) \) has a zero diagonal. This, however, implies that \( (P'AP) - I \) is regular which is a contradiction to an eigenvalue equal to one. \( \square \)

By additionally defining a simple trap as a trap which does not strictly contain a trap, [Van Den Hof, 1998] gives an even more specific result:

**VI.5 Proposition**

Let \( A \) be a compartmental matrix. Then one is an eigenvalue of \( A \) of multiplicity \( k > 0 \) if and only if the corresponding system contains \( k \) simple traps.

**VI.5 Reachability and Observability**

As in the previous section we assume in this section that all lifetimes are a priori known. Furthermore we assume that the lifetimes of all subsystems are equal to one. It is easy to see by the inspection of the relevant system matrices and of the results proved below that this precondition means no loss of generality.

**VI.5.1 Reachability**

**Definition:** A system is called reachable if for any state \( x^{(1)} \) there exists an input sequence which transfers the state of the system from zero to \( x^{(1)} \) within finite time.

It is important to remark that this definition, and thus also the results of this section, do not account for the non-negativity of the variables, namely the flows and the stock levels. Results on this topic which are, however, not of a \( \theta \)-generic type can be found, e.g., in [Valcher, 1996] and [Van Den Hof, 1998].

**VI.6 Proposition**

A system is reachable if and only if for any states \( x^{(0)} \) and \( x^{(1)} \) there exists an input sequence which transfers the state of the system from \( x^{(0)} \) to \( x^{(1)} \) within finite time.

It is well known that \((A_0, B_0)\) is reachable if and only if the controllability matrix

\[
(B_0, A_0 B_0, A_0^2 B_0, \ldots, A_0^{m-1} B_0)
\]

has full row rank \( m \).

Clearly, \( \theta \)-genericity is neither necessary nor sufficient for a property to hold generically in general. For generic reachability, however, the following proposition is stated in [Shields and Pearson, 1976].

**VI.7 Proposition**

A system structure \([A, B]\) is generically reachable if and only if there exists a system \((A_0, B_0) = [A, B]_{d_0}\), where \( d_0 \) is reachable.
Proof: The necessity part is clear from the definition of a proper algebraic set. For the sufficiency part consider the polynomial \( g \in \mathbb{R}[x_1, \ldots, x_r] \) which is defined as the sum of squares of all maximal order minors of the controllability matrix

\[
(B, AB, A^2B, \ldots, A^{m-1}B).
\]

Thus the set

\[
V = \{ d \in N : d \text{ is not reachable} \}
\]

(VI.4)

coincides with the algebraic set defined by the set of zeros of \( g \). By assumption there exists a \( d_0 \in N \setminus V \), so that \( V \) is proper. \( \square \)

Since then generic unreachability is equivalent to \( V = N \) with \( V \) defined as in (VI.4), we immediately have the following\(^2\)

VI.8 Proposition
If \([A, B, \theta] \) is \( \theta \)-reachable for a paramaterisation \( \theta \) then \([A, B] \) is generically reachable.

With the help of the following results it will be shown that in our case, i.e. with parametrisation \( \theta_1 \), the reverse holds as well. Before that, however, a statement analogous to proposition VI.7 will be formulated, which may be proved in the same way as its analogue, if the fact that \( \theta_1 \) is polynomial is taken into account.

VI.9 Proposition
A system structure \([A, B, \theta_1] \) is \( \theta_1 \)-reachable if and only if there exists a system \((A_0, B_0) = [A, B, \theta_1]_{d_0} \) where \( d_0 \) is reachable.

VI.10 Lemma
A system structure \([A, B] \) is generically reachable if and only if the following conditions are satisfied:

A1: The system graph \( \mathcal{G} \) is input-connectable.

A2: On the system graph \( \mathcal{G} \) there exists a family of disjoint cycles and stems such that all vertices in the graph are covered.

Remark 1: This is a reformulation of the central theorem in [Shields and Pearson, 1976], which can be found in [Murota, 1987] and in [Reinschke, 1988], see also [Davison, 1977]. Note that A2 is equivalent to the condition that the generic rank of \([A, B] \) equals \( m \), the dimension of \( A \). The family of disjoint cycles and stems required by the condition A2 is not unique in general. \(<i>\)

Remark 2: It is clear from the construction of the extended graph \( \tilde{\mathcal{G}} \) that the conditions A1 and A2 hold with respect to \( \mathcal{G} \) exactly if they hold with respect to \( \tilde{\mathcal{G}} \). \(<i>\)

Note that a system which is strongly connected (and has - system theoretic - inputs and outputs) is always input- and output-connectable.

VI.11 Proposition
If \([A, B] \) is generically reachable then there exists a system \( d_0 \in S = \theta_1(P) \) which is reachable.

\(^2\)Note that thus \([A, B] \) is generically unreachable if and only if it is not generically reachable.
VI.5 Reachability and Observability

Proof: We will construct a reachable system $(A_0, B_0) = [A, B]_{d_0}$ with $d_0 \in S$, where $S$ is the domain of $\theta_1$. Since we have generic reachability there exists according to condition A2 a family $\mathcal{F}$ of disjoint cycles and stems. Now choose $d \in N$ such that all edges not present in $\mathcal{F}$ vanish, i.e. the corresponding elements of $(A_0, B_0)$ are set to zero.

In the case where $\mathcal{F}$ contains no cycles the elements of $(A_0, B_0)$ corresponding to the edges and imports involved in $\mathcal{F}$ are set to one (so that we remain in $S$). The controllability matrix thus contains all unit vectors $u_i, i = 1, \ldots, m$, since all vertices are covered by $\mathcal{F}$ which in this case consists only of stems.

Now consider a cycle in $\mathcal{F}$. If there is a vertex within the cycle which receives an import then the same argument as before proves reachability, since then the vertices of this cycle can also be covered by a stem. If there is no such vertex then chose a vertex $i$ within the cycle. According to A1 there exists a path from the target of an import to $i$; without loss of generality assume that this path contains no vertices of the considered cycle. Let $j$ be the vertex preceding $i$ in this path. If $j$ is the last vertex of a stem in $\mathcal{F}$ then we are ready, setting the entry of $A_0$ at the $(i, j)$ position equal to one. Otherwise there exists a vertex, $k$ say, succeeding $j$ in one of the stems and cycles in $\mathcal{F}$. If $k$ is covered by a cycle then consider this cycle as before. Going back successively in this way we finally come to either a stem or a cycle which directly receives an import. In any case set the $(i, j)$-element of $A_0$ equal to $\alpha \in (0, 1)$ and the $(k, j)$-element to $1 - \alpha$, thus we remain in $S$. It is then easy to see that the columns of the resulting controllability matrix can be transformed (by a non-singular column transformation) to contain all unit vectors. □

VI.12 Theorem

$[A, B, \theta_1]$ is $\theta_1$-reachable if and only if $[A, B]$ is generically reachable.

Proof: It remains to show the sufficiency part. Thus we assume that $V$ as defined in (VI.4) is a proper algebraic subset of $N$. Since $\theta_1$ is polynomial also $S$ is algebraic (and even proper if $s < r$), so that $W = V \cap S$ is also algebraic in $N$ and in $S$:

$$W = \{d \in S : g_1(d) = 0, \ldots, g_l(d) = 0\}$$

Again because of the fact that $\theta_1$ is polynomial, $U = \theta_1^{-1}(W)$ is thus algebraic in $P$:

$$U = \{p \in P_1 : (g_1 \circ \theta_1)(p) = 0, \ldots, (g_l \circ \theta_1)(p) = 0\}$$

where $g_j \in \mathbb{R}[x_1, \ldots, x_r], j = 1, \ldots, l$. By proposition VI.11 there exists a system $d_0 \in S \setminus W$ (so that $W$ is proper) and therefore also a parameter $p_0 \in P_1 \setminus U$ with $\theta_1(p_0) = d_0$, so that $U$ is proper. □

Remark: Note that the following two properties of $\theta_1$ have been sufficient for being able to prove the sufficiency part of the theorem (proposition VI.11 and theorem VI.12). First $\theta_1$ is polynomial and secondly it is possible to construct, on the basis of a subgraph consisting of a family of disjoint stems and cycles, a reachable system which lies in $[A, B, \theta_1]$ (see the proof of proposition VI.11); examples which show that the latter is not the case in general is given in [Reinschke, 1988]; cf. also section VII.3. □

VI.13 Corollary

$[A, B, \theta_1]$ is $\theta_1$-reachable if and only if conditions A1 and A2 are both satisfied.
Note that A1 and A2 are graph theoretic and therefore generic conditions while the result is of \( \theta \)-generic nature. This means that \( \theta \) describes a class of matrices for which the generic and the \( \theta \)-generic rank coincide, cf. section 2.2 in [Murota, 1987]. Thus we are now able to characterise and interpret the typical \( \theta \)-unreadable material flow systems. The first type of unreadability for the parametrisation \( \theta_1 \), corresponding to condition A1, occurs whenever there is a dynamic subsystem whose stock(s) is (are) only depleted within the given system boundaries, i.e. there is no accumulation. The second type refers to input-connectable but unreadable systems, corresponding to condition A2, and is characterised by a single compartment, \( j \) say, which feeds more than one subsystem such that these subsystems receive no imports and are not contained in cycles which do not contain \( j \) as well.

On the other hand it is possible to characterise a \( \theta_1 \)-reachable system as a system where each subsystem is either part of a circulation of material or part of a chain of material transfer starting with an import. In addition the cycles and stems described in this way must be disjoint.

Before showing another approach to the \( \theta \)-reachability problem, we like to stress the following observation: According to the above results the graph associated with a system structure \([A,B]\), which is not reachable, does not fulfill A1 or A2. Only in the first case, however, it is possible to transform the system structure by simultaneous row and column permutations (which mean a simple renumbering of the subsystems giving an isomorphic system graph) to the standard form of unreadable systems (see Kalman’s Decomposition Theorem, e.g. in [Antsaklis and Michel, 1997]). This means that there exists a permutation matrix \( Q \) such that

\[
[QAQ^{-1},QB] = \begin{bmatrix}
A_{11} & A_{12} \\
0 & A_{22}
\end{bmatrix}
\]  

(VI.5)

If A2 is not satisfied then more general transformations are needed in order to achieve this standard form (cf. proposition VI.29).

Inspired by [Hayakawa et al., 1984] we will specialise the lemma VI.14 by [Corinflat and Morse, 1976] for a compartmental model with parametrisation \( \theta_1 \). Note that the resulting necessary and sufficient conditions for reachability directly refer to \( \theta \)-generic reachability.

Let the matrices \( A \) and \( B \) be parameterised in the following way, defining a class of parameterisations, \( \Theta \) say:

\[
A = A^0 + \sum_{i=1}^{k} B^i P^i C^i 
\]  

(VI.6)

\[
B = B^0 + \sum_{i=1}^{k} B^i P^i D^i,
\]  

(VI.7)

where the elements of \( P^1,\ldots,P^k \) are assumed to be independently varying parameters, and the matrices \( A^0, B^0, B^i, C^i \) and \( D^i \) are fixed and independent of the elements of the \( P^i \). For a given parameterisation \( \theta \in \Theta \) define the graph \( \Gamma_\theta \) with vertices \( i = 0,\ldots,k \) and edges from vertex \( j \) to vertex \( i \) whenever any element of

\[
H^{ij}(\lambda) = \begin{cases}
C^i(\lambda - A^0)^{-1} B^j & i,j \in \{1,\ldots,k\} \\
C^i(\lambda - A^0)^{-1} B^j + D^i & i \in \{1,\ldots,k\}, j = 0
\end{cases}
\]  

(VI.8)
is not identically zero ($\lambda$ is an indeterminate).

Let $K = \{1, \ldots, k\}$. For $S$ containing the indices $i_1, \ldots, i_q$ we define

$$B^S = (B^{i_1}, \ldots, B^{i_q})$$

Similarly, $C^{K \setminus S}$ and $D^{K \setminus S}$ denote the matrices consisting of the matrices $C^i$ and $D^i$, respectively, corresponding to the complementary index set of $S$.

**VI.14 Lemma**

*The system structure $[A, B, \theta]$ with $\theta \in \hat{\Theta}$ is $\theta$-reachable if and only if the following conditions are satisfied:*

**B1:** The graph $\Gamma_{\theta}$ is input-connectable.

**B2:** For all $\lambda$ in the (complex) spectrum of $A^0$ we have

$$\text{rank} \begin{pmatrix} \lambda I - A^0 & B^0 & B^S & D^{K \setminus S} & 0 \end{pmatrix} \geq m \forall S \subseteq K,$$

(VI.9)

We will now show that the system matrices associated with a system parameterised by $\theta_1$ can be represented as in (VI.6) and (VI.7). For this purpose let $n^+(j)$ denote the number of outflows of subsystem $j$ and $\bar{n}^+(j)$ the number of outflows of subsystem $j$ which are no exports. Then the set of subsystems $V$ is partitioned as follows:

- $j \in V_{(i)} \iff n^+(j) > \bar{n}^+(j) > 0$
- $j \in V_{(ii)} \iff n^+(j) = \bar{n}^+(j) > 1$
- $j \in V_{(iii)} \iff \bar{n}^+(j) = 0$
- $j \in V_{(iv)} \iff n^+(j) = \bar{n}^+(j) = 1$

Set $k_{(i)}$ equal to $|V_{(i)}|$, and so on. Furthermore assume, without loss of generality, that the first $k_{(i)}$ subsystems belong to $V_{(i)}$, subsystems $k_{(i)} + 1$ to $k_{(ii)}$ to $V_{(ii)}$ and so on.

**VI.15 Proposition**

*The parameterisation $\theta_1$ is an element of the class $\hat{\Theta}$.***

**Proof:** First note that the import matrix $B$ contains no free parameters, since there are no static subsystems. Since the only columns of matrix $A$ which contain free parameters are those which correspond to the elements of $V_{(i)} \cup V_{(ii)}$, we have $k$ equal to the number of subsystems with more than one outflow and at least one outflow not going to the surroundings, i.e. $k = k_{(i)} + k_{(ii)}$.

Let $l_i(j), i = 1, \ldots, k$ denote the target subsystem of the $i$-th outflow of subsystem $j$ which is not an export or, for $j = 0$, of the $i$-th import, respectively. Then we have for the $j$-th column $a^o_j$ of $A^0$:

$$a^o_j = \begin{cases} 0 & j \in \{1, \ldots, k_{(i)}\} \\ u_{l_{+}^+(j)}(j) & j \in \{k_{(i)} + 1, \ldots, k_{(ii)}\} \\ 0 & j \in \{k_{(ii)} + 1, \ldots, k_{(iii)}\} \\ u_{l_i(j)} & j \in \{k_{(iii)} + 1, \ldots, k_{(iv)}\} \end{cases}$$

where $0$ and $u_i$ denote the zero vector and the $i$-th unit vector, respectively, of appropriate dimension. Furthermore we have

$$B^l = \begin{cases} (u_{l_1(j)}, \ldots, u_{l_{+}^+(j)}(j)) & j \in \{0, \ldots, k_{(i)}\} \\ (u_{l_1(j)} - u_{l_{+}^+(j)}(j), \ldots, u_{l_{+}^+(j)}(j) - u_{l_{+}^{+}(j)}(j)) & j \in \{k_{(i)} + 1, \ldots, k_{(ii)}\} \end{cases}$$
such that $B^0 = B$. In our case $P^j$ is a vector containing the transfer coefficients associated with the outflows of subsystem $j$. Finally we have $C^i = u', i = 1, \ldots, k$ and $D^i = 0', i = 1, \ldots, k$. □

For technical reasons in the context of the definitions and proofs below we need to define a selection of last outflows. By this we mean that for each element of $V_{(\overline{i})}$ or $V_{(\overline{iv})}$ we mark (for an element of $V_{(\overline{iv})}$ there is, of course, only one possibility). It is clear that this selection is not unique. For a given selection of last outflows we mean by an $l$-path a path the edge set of which only consists of last outflows. Note that such a selection has implicitly been performed in the above proof, i.e. the shape of the graph $\Gamma_{\theta_1}$ depends on the selection of last outflows, $L$ say. Thus we have

$$\Gamma_{\theta_1} = \Gamma_{\theta_1}(L)$$

Now define a graph $\tilde{\Gamma}$ with vertices $i = 0, \ldots, k$, where $k$ denotes the number of subsystems with more than one outflow and at least one outflow not going to the surroundings, and edges defined as follows: For vertex $j$ representing a subsystem with at least one export as well as for $j = 0$ there is an edge from vertex $j$ to vertex $i$ if and only if, in $G$, there is an edge from $j$ to $i$ or there is an $l$-path from a successor of $j$ to $i$. For other $j$ there is an edge from $j$ to $i$ in $\tilde{\Gamma}$ if and only if there is an edge from $j$ to $i$ in $G$ or there is an $l$-path in $G$ from one successor of $j$ to $i$, but also another successor of $j$ from which there is no $l$-path of the same length to $i$.

This means that $\tilde{\Gamma}$ consists of the graph $G$ restricted to the first $k_{(i)} + k_{(j)}$ vertices and the surroundings and certain additional edges (exports may be neglected here). Obviously, the location of these additional edges strongly depends on the selection of last outflows, giving

$$\tilde{\Gamma} = \tilde{\Gamma}(L)$$

We can, however, show the following result:

VI.16 Proposition

Let $i, j \neq 0$ be two vertices in $\tilde{\Gamma}(L)$. The property that there exists a path in $\tilde{\Gamma}(L)$ from $j$ to $i$ is independent of the selection of last outflows $L$.

Proof: It is obvious that we may, without loss of generality, assume here that $V_{(\overline{i})}$ is empty. Consider two selections of last outflows, $L_1$ and $L_2$ say, and a path $p$ from $j$ to $i$ in $\tilde{\Gamma}(L_1)$. The part of $p$, which consists of edges each of which directly corresponds to an edge in $G$, can also be found in $\tilde{\Gamma}(L_2)$. Assume therefore that there is an edge in $p$ which corresponds to an $l$-path $p_l$ in $G$, and denote the initial and the terminal vertex of this edge by $l$ and $k$, respectively. We will now construct a path $p_{kl}$ from $l$ to $k$ in $\tilde{\Gamma}(L_2)$. In general, $p_{kl}$ consists of three parts: The first part, from $l$ to $i_1$, say, and the last part, from $i_4$ to $k$ say, involve only elements of $V_{(\overline{i})} \cup V_{(\overline{j})}$. The part in between, i.e. from $i_2$, the successor of $i_1$, to $i_3$, the predecessor of $i_4$, involves only elements of $V_{(iv)}$ such that the corresponding outflows are last outflows also in the case of $L_2$. It remains to consider the edge from $i_1$ to $i_2$. If this edge is a last outflow also in the case of $L_2$ then $p_{kl}$ consists of an edge which corresponds to an $l$-path from the predecessor of $i_1$ to $i_4$ and the remaining edges being the same as in $p_l$. Otherwise $p_{kl}$ consists of an edge which corresponds to an $l$-path from $i_1$ to $i_4$ and the remaining edges being the same as in $p_l$. □

VI.17 Proposition

For a system with a given selection of last outflows $L$ the graph $\Gamma_{\theta_1}(L)$ is isomorphic to the graph $\tilde{\Gamma}(L)$. 

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Proof: First note that $A^0$ is the adjacency matrix associated with the graph $(V,L)$. Next, considered generically for $\lambda$, the summands in

$$(\lambda I - A^0)^{-1} = \frac{1}{\lambda} \left( I + \frac{A^0}{\lambda} + \frac{(A^0)^2}{\lambda^2} + \ldots \right) \quad (VI.10)$$

cannot cancel each other. The $(i,l)$-element of (VI.10) is therefore different from zero if and only if $i = l$ or if there exists a $q \geq 1$ such that the $(i,l)$-element of $(A^0)^q$, which we denote by $(a_{i,l}^0)^q$, is different from zero. The second case means that there is an $l$-path from $l$ to $i$. First assume $j \in \{0,\ldots,k_{(i)}\}$. Then $H^{ij}(\lambda)$ selects the $(i,h(j))$- to the $(i,l_{\sigma(i,j)}(j))$-elements, so that it is different from zero if and only if there exists a $v \in \{1,\ldots,\bar{n}^+(j)\}$ such that the $(i,l_{v}(j))$-element of (VI.10) is different from zero.

For $j \in \{k_{(i)} + 1,\ldots,k_{(i)}\}$ note that $H^{ij}(\lambda) \neq 0'$ if and only if there exists a $v \in \{1,\ldots,\bar{n}^+(j) - 1\}$ and a $q \geq 0$ such that

$$(a_{i,l_v(j)}^0)^q = (a_{i,l_{\sigma(i,j)}(j)}^0)^q$$

Since by construction $(A^0)^q$ for $q \geq 0$ contains only zeroes and ones the proof is finished. \(\square\)

The aim of the following theorem is to translate the conditions B1 and B2 for systems parameterised by $\theta_1$ into graph theoretic conditions. First, because of proposition VI.17, B1 may equivalently be formulated with $\tilde{\Gamma}$ instead of $\Gamma_{\theta_1}$ (see condition C1 below), the definition of the former is more closely related to the system graph $G$. Secondly, note that by construction

$$\text{rank} \left( C^{K\setminus S}, D^{K\setminus S} \right) = k - |S| \quad \forall S \subseteq K,$$

holds so that (VI.9) for $\lambda = 0$ is equivalent to

$$\text{rank} \left( A_{-K\setminus S}^0, B_{-K\setminus S}^0, B^S \right) \geq m - k + |S| \quad \forall S \subseteq K, \quad (VI.11)$$

where $A_{-K\setminus S}^0$ denotes the matrix consisting of all columns of $A^0$ except those corresponding to the complementary index set of $S$. This rank has an obvious and pretty interpretation (see the condition C2 below). However, a cycle of last outflows of length $l$ (which clearly has to be a simple cycle) yields the $l$-th unit roots as eigenvalues of $A^0$. Instead of showing that (VI.11) implies that the analogous condition holds for all $\lambda$ in the spectrum of $A_0$, we will directly prove the equivalence of the resulting conditions in the theorem below with the conditions A1 and A2. In particular note that A1 implies C1 and that A2 and C2 are equivalent.

**VI.18 THEOREM**

A system with parametrisation $\theta_1$ is $\theta_1$-reachable if and only if the following conditions are satisfied:

**C1:** The graph $\tilde{\Gamma}$ is input-connectable.

**C2:** For all $S \subseteq K$ there exist $m - k + |S|$ different subsystems in $G$ each of which is either the target of an import or the successor of a subsystem with index $i \in S \cup V_{(i)}$.

Remark: Note that by proposition VI.16 the condition C1 may indeed be formulated independently of the selection of last outflows. Furthermore the condition C2 obviously does

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not depend on such a selection either, as can also be seen by inspecting the matrices $A^0_{-K\setminus S}$ and $B^S$ in (VI.11).<

**Proof:** A1 $\Rightarrow$ C1: We have to show that an input-connectable system graph $\mathcal{G}$ implies the corresponding graph $\bar{\mathcal{G}}$ is input-connectable as well. For vertex $i \leq k$ denote the vertices of an input-connecting path $\pi$ in $\mathcal{G}$ by

$$i_0 = 0, i_1, \ldots, i_{l-1}, i_l = i$$

If for $j \leq l - 1$ both $i_j \leq k$ and $i_{j+1} \leq k$ hold, then by construction there are two cases:

1. If, as a special case, all outflows of $i_j \in V_{(i)}$ go to $i_{j+1}$ then also the last outflow is among them so that we act as if $i_j$ had a number greater than $k$. Otherwise there is also an edge between them in $\bar{\mathcal{G}}$. For general $i_j$, $i_{j+1}$ denote by $i_p, p \leq j$, and $i_q, q \geq j+1$ the first (going back from $i_j$ or going forward from $i_{j+1}$, respectively) vertices with a number smaller than or equal to $k$. Note that the subsystems $i_j$ for $p < j < q$ necessarily are elements of $V_{(iv)}$ (or, in the special case treated above, of $V_{(iii)}$) and thus the subpath of $\pi$ connecting $i_{p+1}$ to $i_q$ is an $l$-path. Therefore it is straightforward to see that there is an edge in $\bar{\mathcal{G}}$ from $i_p$ to $i_q$. In the special case when $i_p \in V_{(ii)}$ and when there are $l$-paths of the same length from all successors of $i_p$ (one of it being the target subsystem of the last outflow) to $i_q$ then we have an $l$-path from $i_p$ to $i_q$ and we can go back to the first vertex with a number less than or equal to $k$ preceding $i_p$ in $\pi$ as before.

A2 $\Rightarrow$ C2: Assume $\neg C2$ and denote the first $k$ columns of $A^0$ by $X^0$ and the remaining submatrix by $Y^0$, so that $A^0_{-K\setminus S} = (X^0, Y^0)$, where $X^0$ is the matrix consisting of those columns of $X^0$ the indices of which are elements of $S$. Analogously the partitioning $A = (X, Y) = (X^0, Y^0)$ is defined. Thus we have (see proof 1)

$$\neg C2 \iff \exists S \subseteq K : \text{rank}(X^0_S, Y^0, B^0, B^S) < m - k + |S|$$

Denote this element of $\bar{K}$ by $S^*$. Then we have

$$g - \text{rank}(A, B) = g - \text{rank}(X, Y^0, B^0)
= g - \text{rank}(X_{K\setminus S^*}, Y^0, B^0, X_{S^*})
\leq g - \text{rank}(X_{K\setminus S^*}) + g - \text{rank}(Y^0, B^0, X_{S^*})
< (k - |S^*|) + (m - k + |S^*|)
= m$$

For the second inequality note that $g\text{-rank}(X_{S^*}) \leq \text{rank}(X_{S^*}, B^S)$. C1 $\land$ C2 $\Rightarrow$ A1: It is obvious that C1 implies that $\mathcal{G}_{|V_{(i)} \cup V_{(a)}}$ is input-connectable. Assume therefore that there exists a subsystem $i \in V_{(iii)} \cup V_{(iv)}$ which is not input-connectable in $\mathcal{G}$. If it is possible to go back in $\mathcal{G}$ from $i$ to a subsystem in $V_{(i)} \cup V_{(ii)}$ then C1 cannot be satisfied. Otherwise it must be possible to go back in $\mathcal{G}$ to a subsystem $j \in V_{(iv)}$ (or $j = i$ holds) which does not receive an inflow from the surroundings nor from the rest of the system (the case of $j$ being part of a cycle leads to a contradiction to stability in the case of a cycle involving only subsystems in $V_{(iv)}$ or otherwise to a contradiction to C1). With $S = K$ we see that C2 cannot be satisfied.

C2 $\Rightarrow$ A2: C2 can be reformulated as follows: (a) there exists a set $R$ of subsystems, which receive an import or are successors of $V_{(iv)}$, with $r = |R| \geq m - k$ elements, and (b) for all $S \subseteq K$ with $|S| > r - m + k$ there exist $|S| - (r - m + k)$ different subsystems not contained in $R$ each of which is the successor of an element of $S$. Now construct a bipartite graph
where the partition classes \( V^+ \) and \( V^- \) of vertices correspond to \( K \) and \( V \setminus R \), respectively, and an edge from \( i \in V^+ \) to \( j \in V^- \) whenever there is an edge from \( i \) to \( j \) in \( G \). According to corollary II.3 condition (b) is sufficient for the existence of a maximal matching on \( K \) for 
\[
|K| - (r - m + k) = m - r = |V \setminus R| \quad \text{elements.}
\]
Thus it is possible to find a set of edges in \( G \) such that each subsystem not contained in \( R \) is directly influenced by a different subsystem contained in \( K \). Together with (a) this yields a family of disjoint stems and cycles covering all vertices of \( G \). □

### VI.5.2 Observability

**Definition:** A system is called observable if its present state can be determined from knowledge of the present and future outputs and inputs.

The matrix pair \((A_0, C_0)\) is observable if and only if the observability matrix

\[
\begin{pmatrix}
C_0 \\ C_0 A_0 \\ C_0 A_0^2 \\ \vdots \\ C_0 A_0^{m-1}
\end{pmatrix}
\]

has full column rank \( m \).

It is well known (see, e.g., [Antsaklis and Michel, 1997]) that observability, and thus also generic observability, is a dual concept to (generic) reachability. This fact immediately leads to the following dual counterpart of lemma VI.10:

#### VI.19 Lemma

A system structure \([A, C]\) is generically observable if and only if the following conditions are satisfied:

\( \textbf{A1*}: \text{The system graph } G \text{ is output-connectable.} \)

\( \textbf{A2*}: \text{On the system graph } G \text{ there exists a family of disjoint cycles and output stems such that all vertices in the graph are covered.} \)

In the same way it is possible to transfer the results which have lead to theorem VI.12 to the case of observability. Only the analogue of proposition VI.11 requires a closer look since this is the place where the restriction comes in that the non-zero entries of the observation matrix, which correspond to internal flows, are identical to according entries of \( A \):

#### VI.20 Proposition

If \([A, C]\) is generically observable then there exists a system \( d_0 \in S = \theta_1(P) \) which is observable.

**Proof:** Consider a family \( \mathcal{F} \) of disjoint cycles and output stems based on which we will construct an observable system \((A_0, C_0) = [A, C]_{d_0}\) with \( d_0 \in S \). Because of the above mentioned restrictions on the entries of the state transformation and the observation matrix we have to take care of the output stems in \( \mathcal{F} \): As in the case of reachability (cf. the proof of proposition VI.11), all involved edges lead to corresponding one entries in \( A_0 \), the involved outputs, however, give one entries in \( C_0 \) and thus also ones at the corresponding
positions in $A_0$. The same is true for the outputs or output stems used to observe the cycles in $F$. It is straightforward to see that these additional non-zero entries in $A_0$ do not reduce the rank of the observability matrix in comparison to the case where the restrictions are not taken into account, since each output stem brings in only one new edge represented in $A_0$. □

Thus the main results of this section can be formulated:

VI.21 Theorem
$[A, C, \theta_1]$ is $\theta_1$-observable if and only if $[A, C]$ is generically observable.

VI.22 Corollary
$[A, C, \theta_1]$ is $\theta_1$-observable if and only if conditions $A1^*$ and $A2^*$ are both satisfied.

VI.5.3 Minimality

Definition: A system represented by $(A, B, C)$ is called minimal if the associated state space dimension $m$ is minimal among all observationally equivalent systems.

Observationally equivalent systems are defined to have the same transfer function. Two minimal systems $(A, B, C)$ and $(\hat{A}, \hat{B}, \hat{C})$ have the same transfer function exactly in the case when there exists a non-singular matrix $Q$ such that $\hat{A} = QAQ^{-1}$, $\hat{B} = QB$ and $\hat{C} = CQ^{-1}$ hold.

VI.23 Proposition
A system represented by $(A, B, C)$ is minimal if and only if $(A, B)$ is reachable and $(A, C)$ is observable.

Now it is important to see that the above definitions are problematic in the structural case (see section VI.2). First it is not clear in which way the above mentioned transformations between observationally equivalent minimal systems have to be restricted in order to be in accordance with the (structural) a priori information. Furthermore, in most structural cases, as in ours\(^3\), the state dimension is also part of this a priori information (cf. [Travis and Haddock, 1981]), so that it is not at all natural to restrict further investigations on, e.g., identifiability to minimal systems.

From theorem 14.5 in [Reinschke, 1988] and the two preceding subsections we get the following characterisation of systems that are both $\theta_1$-reachable and $\theta_1$-observable:

VI.24 Theorem
$[A, B, C, \theta_1]$ is $\theta_1$-reachable and $\theta_1$-observable if and only if the following two conditions are met:
(i) The system graph $\mathcal{G}$ is input- and output-connectable.
(ii) On the system graph $\mathcal{G}$ there exists a family of disjoint cycles and paths from the target of an input to the source of an output such that all vertices in the graph are covered.

Remark: Note that the non-trivial part of the theorem - as a consequence of the theorems VI.12 and VI.21 - is the fact that the existence of a family of disjoint cycles and stems as well as of a family of disjoint cycles and output stems guarantees condition (ii). <

\(^3\)Note, however, that in general compartmental systems this is not always the case, see the discussion in chapter IV.
VI.6 Identifiability

In this section we will find conditions for the model parameters, which in the case of exact lifetimes coincide with the transfer coefficients, to be uniquely reconstructable from perfect flow data. These conditions are based on the a priori information given by the system graph, the non-negativity constraints and the balance requirements for each subsystem. The starting point of our approach is a graph theoretic interpretation of the coefficients of the transfer function⁴, see [Audoly and D’Angio, 1983].

DEFINITION: A system of a given model class is \( \theta \)-generically (globally) identifiable or \( \theta \)-identifiable if the function which maps the non-negative free parameters to the space of transfer functions is injective for all choices of the free parameters except on an algebraic set.

As already mentioned in section VI.2 this definition has an implicit structural character in the sense of [Hannan and Desoete, 1988]. In addition note that this definition implicitly relies on zero initial states. Identifiability from the Markoff parameters and the initial states is discussed in [Van Den Hof, 1998].

The notion of identifiability used here is often called a priori identifiability. Together with questions of data collection, experimental design, the choice of an appropriate compartmental structure (see chapter IV) and parameter estimation this is called the inverse problem, see [Jacquez, 1972]. It has been stated by many authors since the seventies that a general solution for the identifiability problem is still missing. Often only some special cases are treated such as mamillary systems or catenary systems in [Cobelli et al., 1979b]. In most studies restrictions on the input or the observation matrix are imposed, often only the trivial parameterisation is investigated and the resulting conditions are either only sufficient or only necessary. In order to list some of the alternatives to the transfer function approach, most of which deal with the continuous-time case, we mention exhaustive modelling, see [Walter, 1982], an approach via normal modes, see [Norton, 1980], and the use of the norm-coerciveness theorem in [Delforge et al., 1986]. An overview is given in the introduction of [Norton, 1982]. [Godfrey and Chapman, 1990] and [Zhang et al., 1991] present geometric (i.e. graph theoretic) rules for the transformation between different observationally indistinguishable compartmental structures.

The graph theoretic identifiability conditions presented in this chapter are necessary and sufficient and treat a rather general model class, which is given by the parameterisation \( \theta_1 \).

VI.6.1 Graph Theoretic Description of the Transfer Function

It will now be shown that the coefficients of the transfer function (often called moment invariants) of a \( \theta_1 \)-parameterised system can be described by forms and reduced forms (as introduced by [Audoly and D’Angio, 1983], see chapter II), of the system graph \( G \). These quantities are polynomials in the edge weights of \( G \), i.e. in the transfer coefficients. For clarity of notation the following result is proved for the case where all lifetimes are equal to one. The general case will be stated as a corollary. For this purpose we introduce the convention that the length of a (generalised) cycle on the system graph means the sum of the lifetimes of the involved subsystems and the length of a (generalised) path means the sum of the lifetimes of the involved subsystems minus one (since the length of a path equals the number of its edges). In addition it is important to keep in mind that subsystems with lifetime \( \tau_i > 1 \) are modelled as a chain of \( \tau_i \) subsystems each of which has a lifetime equal

⁴It is equivalent to define identifiability via the transfer function and to define it via the Markoff parameters.
to one. Thus in the corollary the lengths of the cycles and paths refer to the extended graph $\tilde{G}$ which includes these chains.

With $s$ denoting the (forward) shift operator, the transfer function is given as

$$k(s) = C(sI - A)^{-1}B$$

Note that this gives a matrix of rational functions in $s$ where all common factors in each entry are cancelled. Following [Kailath, 1980] we call

$$\frac{C(sI - A)^{v}B}{\text{det}(sI - A)} \quad (VI.12)$$

where, for a non-singular matrix $L$, $L$ denotes its cofactor matrix (or, equivalently, the transpose of its adjoint), the nominal transfer function, in which no cancellations have taken place. In the following we will call the paths from the initial subsystem of an input to the terminal subsystem of an output the input-output paths.

**VI.25 Proposition**

Consider an input $e_i$ and an output $e_j$ in a $\beta_1$-parameterised system with $\tau_i = 1 \forall i = 1, \ldots, m$. Then the denominator of the nominal transfer function is given by

$$s^{m} + \sum_{l=0}^{m-1} (-1)^{m-l} \varphi_{V}^{(m-l)} s^{l} \quad (VI.13)$$

and the $(j, i)$-entry of the numerator is given by

$$t_j \left( s^{m-1} + \sum_{l=0}^{m-2} (-1)^{m-l-1} \varphi_{V}^{(m-l-1)} s^{l} \right) \text{ for } t(e_i) = s(e_j)$$

$$t_j \sum_{l=0}^{m-2} (-1)^{m-l} \rho_{s(e_j), t(e_i)} s^{l} \text{ for } t(e_i) \neq s(e_j) \quad (VI.14)$$

**Proof:** By lemma II.8 the determinant of $L$ can be computed as

$$\text{det}(L) = (-1)^{m} \sum_{c^{(m)}} (-1)^{\gamma(c^{(m)})} \omega(c^{(m)}) \quad (VI.15)$$

where the sum is ranges over all generalised cycles $c^{(m)}$ of length $m$. $\omega(\cdot)$ and $\gamma(\cdot)$ denote the weight of and the number of cycles in the considered generalised cycle. The matrix which we consider here is the matrix $(sI - A)$ where $A$ is the adjacency matrix associated with the system graph $\tilde{G}$. Then in each summand of (VI.15) the potency of $s$ and the length of the generalised cycle sum up to $m$. Note that now the generalised cycles refer to the graph corresponding to $A$ as will be indicated by the notation $\tilde{c}^{(l)}$, while $c^{(l)}$ shall refer to the graph corresponding to $(sI - A)$. By taking into account (II.1) for the potency of $(-1)$ we have

$$\varphi_{V}^{(l)} = \sum_{\tilde{c}^{(l)}} (-1)^{l+\gamma(\tilde{c}^{(l)})} \omega(\tilde{c}^{(l)})$$

where the sum is taken over all generalised cycles (with respect to $A$) of length $l$. Since a potency for $s$ of $l$ means $l$ loops in the considered generalised cycle (with respect to $(sI - A)$) we have

$$\gamma(c^{(m,l)}) = \gamma(\tilde{c}^{(m-l)}) + l$$

50
where \( \ell^{m, l} \) denotes a generalised cycle of length \( m \) including \( l \) loops. Therefore we get

\[
\sum_{l=0}^{m} (-1)^{m-l} s^l \varphi_{\ell}^{(m-l)} = \sum_{l=0}^{m} (-1)^{m-l} s^l \sum_{\ell^{m-l}} (-1)^{m-l+\gamma(\ell^{m-l})} \omega(\ell^{(m-l)}) \\
= \sum_{l=0}^{m} (-1)^{m} \sum_{\ell^{m-l}} (-1)^{\gamma(\ell^{m-l})} \left( s^l (-1)^{m-l} \omega(\ell^{(m-l)}) \right) \\
= \sum_{l=0}^{m} (-1)^{m} \sum_{\ell^{m-l}} (-1)^{\gamma(\ell^{m-l})} \omega(\ell^{(m-l)}) \\
= (-1)^{m} \sum_{\ell^{m}} (-1)^{\gamma(\ell^{m})} \omega(\ell^{(m)})
\]

For the third equality note that each factor in \( \omega(\ell^{m}) \) is either an \( s \) or the negative of an element of the matrix \( A \). The proof for the coefficients in (VI.14) runs analogously, taking into account the observation coefficients in the observation matrix \( C \) gives the stated results. \( \square \)

Note that the proposition shows that \( k(s) \) is strictly proper. Furthermore it is easy to see that, despite the balance equations, the summands in each of the coefficients in (VI.13) and (VI.14) cannot cancel each other to zero \( \theta_1 \)-generically.

**VI.26 Corollary**

Consider an input \( e_i \) and an output \( e_j \) in a \( \tilde{\theta}_1 \)-parameterised system. Let \( T \) denote the sum of all lifetimes. Then the denominator of (VI.12) is given by

\[
s^T + \sum_{l=0}^{T-1} (-1)^{T-l} \varphi_{\ell}^{(T-l)} s^l \tag{VI.16}
\]

and the \((j,i)\)-entry of the numerator is given by

\[
t_j \left( s^{T-t_{(e_i)}} + \sum_{l=0}^{T-t_{(e_i)}} (-1)^{T-t_{(e_i)}-l} \varphi_{\ell}^{(T-t_{(e_i)})} s^l \right) \quad \text{for } t(e_i) = s(e_j) \\
t_j \sum_{l=0}^{T-t_{(e_i)}} (-1)^{T-l} \rho_{(e_j), t_{(e_i)}}^{(T-l)} s^l \quad \text{for } t(e_i) \neq s(e_j) \tag{VI.17}
\]

Thus the power of \( s \) in the case of a non-zero coefficient of the numerator or denominator polynomial equals \( T \) or \( T - t_{(e_i)} \), respectively, minus the sum of the lifetimes of all subsystems (including \( t(e_i) \) and \( s(e_j) \)) which are involved in the corresponding generalised path or cycle.

If a flow \( e_j \) is observed and there is an input \( e_i \) in the same subsystem of which \( e_j \) is an outflow then the coefficient of the linear term of the numerator polynomial is \( t_j \):  

**VI.27 Corollary**

Let \( e_i \) be an input. Then for all observed outputs \( e_j \) of the subsystem \( t(e_i) \) the corresponding transfer coefficient \( t_j \) is identifiable.

**VI.6.2 Common Factors**

Now the question arises in which cases there are transfer coefficients or free parameters (depending on whether we take a generical or a \( \theta \)-generical point of view) which do not
appear in the denominator nor in one of the numerator polynomials of \( k(s) \). Clearly, these cannot be identified from the transfer function. There are two cases to be distinguished: first, there might be flows in the system which are not part of any cycle or of any input-output path (see the definition of \( E_0 \) in the next subsection). Clearly the corresponding transfer coefficients will not even occur in the nominal transfer function (VI.12) and thus neither in (VI.13) nor in (VI.14). Some of these, however, can be identified via the balance equations. The case which we are interested in here occurs when transfer coefficients or free parameters, which a priori do occur in these polynomials, are not involved in the transfer function \( k(s) \) because certain factors in all numerators and the denominator of the nominal transfer function cancel each other.

Such terms will be called common factors\(^5\). If we speak of a \( \theta \)-generic common factor for a parameterisation \( \theta \) this means that the fact that there is such a common factor is \( \theta \)-generic, not that the common factor itself is. It is clear that additional restrictions on the entries of the system matrices may cause additional cancellations. Thus a root which is a common one \( \theta_1 \)-generically need not be so \( \theta_1 \)-generically.

An alternative way of looking at the problem of common factors in the nominal transfer function is to ask whether the coefficients of \( k(s) \) can always be interpreted as generalised cycles or generalised paths of a graph, which is closely related to the system graph. We will start with a simple lemma that gives a first insight.

For \( V_1, V_2 \) being a disjoint decomposition of \( V \) a connecting cycle of \( V_1 \) and \( V_2 \) is a cycle which has at least one vertex in \( V_1 \) and one in \( V_2 \). With this definition a decomposition law for forms of a given length \( l \) can be stated as follows, cf. [Audoly and D’Angio, 1983]: Let \( V_1, V_2 \) be a disjoint decomposition of \( V \). Then we have

\[
\phi_V^{(l)} = \sum_{l_1 + l_2 = l} \phi_{V_1}^{(l_1)} \phi_{V_2}^{(l_2)} + \sum_{1 \leq l_1 \leq l} c_{i_1, \ldots, i_{l_0}} \sum_{l_1 + l_2 = l - l_0} \phi_{V_1}^{(l_1)} \phi_{V_2}^{(l_2)}
\]

where the second summation ranges over all connecting cycles of \( V_1 \) and \( V_2 \) of maximal length \( l \) and \( V_k = V_k \cap V \setminus \{i_1, \ldots, i_{l_0}\} \) for \( k = 1, 2 \).

It is clear from the definition of a strong component that for \( \{G_{V_k}, k = 1, \ldots, r \} \) being the S-decomposition of the system graph \( G \) there are no connecting cycles between \( V_k \) and \( V_{k'} \) with \( k_1 \neq k_2 \). Since also the reverse is true a disjoint decomposition \( \{V_k, k = 1, \ldots, r \} \) of \( V \) is the finest disjoint decomposition without connecting cycles if and only if the \( \{G_{V_k}\} \) are exactly the strong components of \( G \).

**VI.28 Lemma**

Let \( \{G_{V_k}, k = 1, \ldots, r \} \) be the S-decomposition of the system graph \( G \). Then

\[
\det(sI - A) = \prod_{k=1}^{r} \det(sI - A_k)
\]

\[
(sI - A)_{t,s} = (sI - A^{(s,t)})_{t,s} \prod_{k \in R(s,t)} \det(sI - A_k),
\]

where \( R(s,t) \) denotes the index set of all strong components which contain a part of a path from vertex \( t \) to vertex \( s \), and where \( A_k \) and \( A^{(s,t)} \) denote the submatrices of \( A \) corresponding to the subgraphs \( G_{V_k} \) and \( G_{\{V_k, k \in R(s,t)\}} \), respectively. \( s' \) and \( t' \) denote the column and row \n
\(^5\)The notion of a reducible transfer function implicitly defined in this way should not be confused with the more common definition via coprime matrix fraction descriptions, see [Kalish, 1980].
index in $A^{(s,t)}$ which correspond to $s$ and $t$, respectively, for the whole matrix $A$. For $s = t$ the set $R^{(s,s)}$ consists only of the index associated with the strong component containing $s$.

**Proof:** Without loss of generality, assume that the $V_k$ and thus also the $A_k$ are ordered according to the partial ordering defined by the $S$-decomposition. By $k_t$ and $k_s$ denote the indices of the strong components which contain $t$ and $s$, respectively, so that $k_t \leq k \leq k_s$ holds for all $k \in R^{(s,t)}$. Furthermore assume (without loss of generality, since we only have a partial ordering) that for all $k \notin R^{(s,t)}$ with $k > k_t$ also $k > k_s$ holds. This gives

$$sI - A = \begin{pmatrix} sI - A_1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ sI - A_r & \cdots & 0 & sI - A_r \end{pmatrix}$$

Finally note that building the $(t,s)$-element of the cofactor matrix of $sI - A$ is equivalent to computing the determinant of $sI - A$ after replacing the $s$-th column by the $t$-th unit vector, which only affects the part corresponding to $R^{(s,t)}$. $\square$

The next result (see [Cobelli et al., 1979a]) could also be proved with the help of the lemma:

**VI.29 Proposition**

*If a system is $\hat{\theta}_1$-identifiable then its system graph is input- and output-connectable.*

**Proof:** The matrices $A$ and $B$ of a system which is not input-connectable have, without loss of generality, the following block partitioning, cf. (VI.5):

$$(A, B) = \begin{pmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{pmatrix} B_1$$

where the second block row corresponds to the system part which is not input-connectable. Thus we have

$$(I_{s^{-1}} - A)^{-1} = \begin{pmatrix} (I_{s^{-1}} - A_{11})^{-1} & -(I_{s^{-1}} - A_{11})^{-1}A_{12}(I_{s^{-1}} - A_{22})^{-1} \\ 0 & (I_{s^{-1}} - A_{22})^{-1} \end{pmatrix}.$$

It is then easy to see that the parameters in $A_{12}$ and $A_{22}$ do not occur in the transfer function $k(s) = C(I_{s^{-1}} - A)^{-1}B + D$ (even though the second block column of $C$ may contain elements the $A_{22}$). The proof for output-connectability runs analogously. $\square$

Hence, for a system which does not fulfill $A_1$, the transfer coefficients occurring in the part of the system which is represented by the second block row in (VI.18) do not appear in the transfer function (as already mentioned by [Cobelli et al., 1979a] and others). There are no input-output paths running through this part of the system, while its cycles cancel in the denominator and all numerators as indicated by lemma VI.28. For the parametrisation $\hat{\theta}_1$ the situation might occur that, because of the balance equations, there is a transfer coefficient but no free parameter involved in the common factor. This leads to the following result:

**VI.30 Proposition**

*If condition $A_1$ or $A_1^*$ is not satisfied, but both conditions $A_2$ and $A_2^*$ are satisfied, then there exists a $\hat{\theta}_1$-generic common factor which either contains free parameters or is equal to $s^k - 1$ for some $k > 0.*
A Dynamic Model with Exact Lifetime

VI.6 Identifiability

![Diagram](image)

Figure VI.3: Example of a system fulfilling A1, A1*, A2 and A2*, but with $\phi_V^{(m)} = 0$ and $\rho_{m(t(e),t(e_i))}^{(m-1)} = 0$ for all inputs $e_i$ and all outputs $e_j$. Emphasised arrows indicate observed flows.

**Proof:** It remains to explain the special case of a common factor equal to $s^k - 1$. The question is: What does a part of the system look like which involves no free parameters and which corresponds to $A_22$ in (VI.18) or to the corresponding matrix in the output-unconnectable case, respectively? The only possibility is that all transfer coefficients associated with the outflows of the subsystems in that part are equal to one (by the balance equations), i.e. all these subsystems have only one outflow. Now there are two possibilities: First, if A1 is violated then the output-unconnectable part has to be a path from a subsystem without inflows to some subsystem in the part of the system corresponding to A11, because we assume that the system graph is connected. This, however, implies that A2 is not fulfilled either. Thus the second possibility has to be true, namely that there is a simple cycle of unobserved flows which receives inflows from the rest of the system. The transfer function of such a cycle is $(s^k - 1)^{-1}$ so that using the lemma finishes the proof. □

VI.31 Proposition

Let $k(s)$ be the transfer function of a system structure $[A, B, C]$. If one of the conditions $A2, A2^*$ is not satisfied then the denominator polynomial and all numerator polynomials of the nominal transfer function have a $\theta_1$-generic common zero equal to zero.

**Proof:** It is obvious from (VI.13) and (VI.14) that there is a common zero of $\det(sI - A)$ and all elements of $C(sI - A)^TB$ which is equal to zero if and only if $\phi^{(m)}_V = 0$ and $\rho_{m(t(e),t(e_i))}^{(m-1)} = 0$ hold for all inputs $e_i$ and all outputs $e_j$. If one of these conditions is not satisfied then it is easy to construct from the resulting generalised cycle or generalised path, respectively, a family of disjoint cycles and paths as given in condition (ii) of theorem VI.24. □

It is important to see that the reverse of the statement given in proposition VI.31 is not true in general, see the example shown in fig. VI.3. Furthermore, if $A2$ or $A2^*$ is not satisfied common zeroes which are different from zero are not excluded. By the consideration in the beginning of the proof it is easy to see from the system graph whether or not a common factor equal to $s^k, k > 0$, occurs and, if so, to get the maximal value of $k$.

VI.32 Proposition

There is a $\theta_1$-generic common factor equal to $s^k$ with maximal $k > 0$ if and only if $k$ is
the maximal integer such that \( \varphi^{(m-l)}_{\psi} = 0 \) and \( p^{(m-l-1)}_{s(e_j),i(e_i)} = 0 \) hold for all inputs \( e_i \) and all outputs \( e_j \) and for all \( l = 0, \ldots, k - 1 \).

Consequently, in the case addressed in the proposition, the interpretation of the coefficients of the transfer function polynomials via proposition VI.25 is still valid after a corresponding simple modification such that instead of (VI.13) we use

\[
s^{m-k} + \sum_{l=k}^{m-1} (-1)^{m-l} \varphi^{(m-l)}_{\psi} s^{l-k}
\]

and an analogous expression instead of (VI.14).

Let \( \hat{m} \) be the degree of the minimal polynomial associated with \( k(s) \), i.e. the least common denominator of the entries of \( k(s) \), and \( \hat{k} \) the maximal value of \( k \) in the proposition above. With \( m_{\text{con}} \) denoting the number of input- and output-connectable subsystems we give the following

**Definition:** We call the transfer function \( k(s) \) *graphically interpretable* if \( \hat{m} = m_{\text{con}} - \hat{k} \) holds.

### VI.6.3 Graph Theoretic Conditions with Known Lifetimes

The aim of this subsection is to find necessary and sufficient graph theoretic conditions for the identifiability of the model class resulting from the parameterisation \( \vartheta_1 \) for the case where the lifetimes of all subsystems are known a priori. For this purpose, however, we first need some results on the identifiability of systems parameterised by \( \hat{\vartheta}_1 \). Since assumption 2c is not valid under \( \hat{\vartheta}_1 \) we know that each edge which is not an import of the system is assigned an independently varying transfer coefficient, while each import has weight one.

In the remainder of this section we assume that \( k(s) \) is graphically interpretable. Thus the transfer function can be described via (VI.13) and (VI.14) after deleting input- or output-unconnectable parts from the system graph and taking into account proposition VI.32. For simplicity we will formulate all results on identifiability for the case \( \hat{m} = m = m_{\text{con}} \).

Let us now assume that the transfer function of the system under consideration has been estimated (from perfect data), i.e. our starting point is the set of the estimated coefficients \( |\hat{\varphi}_{\psi}^{(l)}| \) and \( |\hat{t}_{\rho_{\gamma}}^{(l)}| \), which we may assume to be consistent with each other\(^6\). From these the transfer coefficients should be identified according to the definitions of generalised cycles and paths. Each *identification equation*, i.e. each equation associated with the identifiability problem, has one of the following forms:

\[
\sum \prod t_j = |\varphi_{\psi}^{(l)}|, \quad \sum \prod t_j = |t_{\rho_{\gamma}}^{(l)}|,
\]

where each sum ranges over all generalised cycles or paths, respectively, of a given length, while the products range over the transfer coefficients corresponding to the edges of the considered generalised cycle or generalised path, respectively, including the transfer coefficient associated with the considered output. The following proposition shows that under assumption 4 we may consider a similar system of equations, the left-hand sides of which consist of only one summand each.

\(^6\)This means that we assume the true model to be contained in the model class.
VI.33 Proposition

Under assumption 4, for a system parameterised by \( \tilde{\theta}_1 \) the identification equations (VI.19) can be reduced to a system of equations

\[
\prod t_j = \hat{\Phi}_j, \quad \prod t_j = \hat{R}_j,
\]

where the products range over the transfer coefficients associated with the cycles and paths of the system graph.

Proof: Consider one of the equations (VI.19) associated with a set of generalised cycles of a given length. By assumption at most one of the summands corresponds to a generalised cycle which consists of only one single cycle. For each of the generalised cycles corresponding to the other summands we now consider sequentially one of the underlying single cycles after the other. Again by assumption, no two of these cycles can enter the same identification equation as a generalised cycle by itself. Thus we may proceed as before with each of these equations. Each branch of this procedure is terminated when a (single) cycle is reached for which there is no generalised cycle of the same length (Obviously, such a terminating cycle has to exist for each branch). For each of the equations related to these terminating cycles we set

\[
\hat{\Phi}_j = |\phi_j|.
\]

Consequently, we can express all the right-hand sides of (VI.20) via those of (VI.19) by calculating along the branches in the reverse direction. The proof for the generalised paths runs quite analogously. \( \Box \)

As a consequence we will, for the remainder of this chapter, assume that the condition 4 is valid and thus consider the equations (VI.20) instead of the equations (VI.19). Otherwise a polynomial or multilinear equation system would have to be solved. This can be done for given systems with the help of computer algebra tools, see, e.g., [Raksanyi et al., 1985], which are often based on Gröbner Bases (see, e.g., [Fröberg, 1997]) or on Cylindrical Algebraic Decomposition (see [Arnon et al., 1984]).

Definition: The cycle matrix consists of the non-negative rows of the semicycle matrix (without loss of generality non-positive rows do not occur).

VI.34 Lemma

Consider a connected graph \( \mathcal{G} \) with \( n \) edges and \( m \) vertices. The kernel of the semicycle matrix is spanned by the incidence cuts, i.e., by the rows of the incidence matrix. The kernel of the cycle matrix is spanned by the incidence cuts and the \( n \)-dimensional unit vectors corresponding to those edges in \( \mathcal{G} \) which are part of a semicycle but of no cycle.

Proof: The first statement follows directly from lemma II.6. Since the cycle matrix consists of rows of the semicycle matrix it is clear that a generator set of its kernel contains the incidences cuts. Therefore the second statement follows from the fact that the columns corresponding to semicycle edges which are not contained in any cycle contain only zeroes. \( \Box \)

Consider a set \( P \) of paths on \( \mathcal{G} \) and let us gather those edges, which are not part of any cycle nor of any path in the given path set \( P \), in \( E_{0,P} \), and let the cardinality of this set be denoted by \( n_{0,P} \).

Motivated by the fact that a cycle and an incidence cut always have an even number of edges in common we give the following
DEFINITION: A vertex $k$ in a graph $G$ with path set $P$ is called critical with respect to $P$ if (i) there is an edge incident to $k$ which is not an element of $E_0.P$ and (ii) for all $p \in P$ the number of edges which are incident to $k$ and at the same time in $E(p)$ is even. The set and the number of critical vertices is denoted by $V^*_P$ and $m^*_P$, respectively.

The reason for the first condition will be clear from the proof of the next theorem below. Note that by the definition of a path the number of common edges mentioned in the definition above equals zero, one or two. From now on, unless stated differently, we will use the path set, $\hat{P}$ say, containing all paths from $t(e_i)$ to $t(e_j)$ via $e_j$ where $e_i$ is an input and $e_j$ is an output and $t(e_i) \neq t(e_j)$. For simplification the set and the number of critical vertices corresponding to this path set will be denoted by $V^*$ and $m^*$, respectively; $E_0$ and $n_0$ are to be understood analogously. Note that $E_0$ contains (among others) all unobserved exports.

It is obvious that for all edges $e_j$ in $E_0$, which are no exports, the vertex $s(e_j)$ is not input-connectable or $t(e_j)$ is not output-connectable. Thus for a strongly connected system $E_0$ contains no internal flows.

We have the following simple and obvious characterisation of critical vertices:

VI.35 Lemma
A vertex $k$ is critical if and only if (i) the first condition of the definition is satisfied and (ii) there is no input $e_i$ for which $t(e_i)$ is contained in a path of $\hat{P}$ and $k = t(e_i)$, and there is no output $e_j$ for which $t(e_j)$ is contained in a path of $\hat{P}$ and $k = t(e_j)$.

Note that the second condition takes care of the fact that only those inputs and outputs are relevant here which indeed are involved in input-output paths. As a counter-example consider a vertex the only observed inflow of which is the only outflow of an input-unconnectable vertex.

In the following it is assumed that the critical vertices have the $m^*$ first numbers and that the edges in $E_0$ have the first indices in $E(G)$.

VI.6.3.1 All Lifetimes are Equal to One
In a first step we consider the case where all lifetimes are equal to one. It will then have to be investigated whether the resulting identifiability conditions are still valid in the general case without having to replace each subsystem by a chain (of appropriate length) of subsystems of lifetime one (cf. fig. VI.2).

The first results below concern the case where the balance equations (assumption 2c) are not taken into account. They will serve as a basis for the proof of the main result.

VI.36 Theorem
A system parameterised by $\hat{b}_1$ is $\hat{b}_1$-identifiable if and only if

$$V^* = E_0 = \emptyset$$

In the unidentifiable case $(m^* + n_0 > 0)$ the solutions of the identification equations are

---

7In general $t(e_j)$ might be reachable from $t(e_i)$ also via another inflow than $e_j$.
8Note that a sequence from $t(e_i)$ to $t(e_j)$ where these two vertices coincide is a cycle and thus, as will be seen below, need not be taken into account in the context of critical vertices.
A Dynamic Model with Exact Lifetime

VI.6 Identifiability

given as

\[
t_j = t_j \left[
\begin{array}{c}
\alpha_{s(e_j)}
\end{array}
\right]
\]

for \( e_j \notin E_0 \), \( s(e_j) \notin V^* \), \( t(e_j) \in V^* \)

\[
\alpha_{s(e_j)}^{-1} \alpha_{t(e_j)}
\]

for \( e_j \notin E_0 \), \( s(e_j) \in V^* \), \( t(e_j) \in V^* \)

\[
\alpha_{s(e_j)}^{-1} \alpha_{t(e_j)}
\]

for \( e_j \notin E_0 \), \( s(e_j) \in V^* \), \( t(e_j) \notin V^* \)

\[
\alpha_{m^*+}.
\]

for \( e_j \in E_0 \), \( s(e_j) \notin V^* \)

\[
1
\]

else

where \( t_j^p \) is a positive particular solution of (VI.20) which is arbitrary for \( e_j \in E_0 \) and otherwise depends on the \( \Phi^{(i)} \) and \( \tilde{R}^{(i)} \) and where the \( \alpha_k \) (\( k = 1, \ldots, m^* + n_0 \)) are the positive real free parameters.

Proof: Consider the coefficient matrix, \( L \) say, of the linear equation system which results from taking the logarithm of the equations (VI.20). Since every edge which is not an input is assigned a transfer coefficient \( L \) has \( n - n_{in} \) columns. There are as many rows as there are generalised cycles and paths. The \((i,j)\)-element is equal to one if the edge \( e_j \) is part of the generalised cycle or path represented in the \( i \)-th row. By the assumption of consistent estimates for the weights of the generalised cycles and paths a solution always exists.

Since we are interested only in the column rank and the (right) kernel of \( L \) we may as well consider the matrix \( L_1 \) the rows of which represent the simple cycles and the paths, since this can be obtained from \( L \) by

\[
\begin{pmatrix}
L_1
L_0
\end{pmatrix} = TL,
\]

where \( T \) is a regular row transformation matrix and the rows of \( L_0 \) are linearly dependent on those of \( L_1 \). Note that the rows of \( L_1 \) are linearly dependent in general. According to Lemma VI.34 the kernel of the cycle matrix is spanned by the incidence cuts and those unit vectors which correspond to semicycle edges that are not contained in a cycle. The edges of this kind which in addition are not contained in any paths (i.e. the corresponding unit vectors are orthogonal to all rows representing paths) are obviously contained in \( E_0 \). Since all columns of \( L \) and therefore of \( L_1 \) which correspond to elements of \( E_0 \) contain only zeroes we have a corresponding unit vector for each element of \( E_0 \) in the basis of the kernel of \( L_1 \).

It therefore remains to select those incidence cuts for completing this basis which are orthogonal to all paths and to all selected unit vectors. This, however, is straightforward since by the definition of the critical vertices the incidence cuts entering the basis of the kernel of \( L_1 \) are exactly those corresponding to the elements of \( V^* \). In order to simplify (in a certain sense) the basis we subtract from each selected incidence cut vector the unit vectors corresponding to elements of \( E_0 \) which are inflows of the considered subsystem. The matrix of the resulting basis vectors now is the incidence matrix of a graph \( G^* \) the vertex set of which consists of \( V^* \), for each element of \( E_0 \) with \( s(e_j) \notin V^* \) an isolated vertex receiving an input and for each other element of \( E_0 \) another vertex. The edges of the system graph with initial or terminal vertex in \( V^* \) are the same in this graph except those in \( E_0 \) with \( s(e_j) \in V^* \) each of which gets as its new terminal vertex the respective vertex representing it.

The solutions of the log-transformed equation system are thus given as

\[
\log(t_j) = \log(t_j^p) + \sum_{k=1}^{m^*+n_0} b_{jk} \log(\alpha_k)
\]

\[
= \log(t_j^p) + \sum_{k=1}^{m^*+n_0} \log(\alpha_k^{b_{jk}}),
\]

58
where $\alpha$ is the vector of parameters according to the degree of freedom and $b_j$ is the $j$-th component of the $k$-th basis vector. It is clear that the particular solutions corresponding to zero columns in $L$, i.e. to elements of $E_0$, can take arbitrary values. By back-transformation and considering the special form of the basis vectors the proof is complete. $\square$

Remark: If the following condition

$$V^* \neq V \text{ or observed exports exist} \quad (*)$$

is not satisfied (the former condition means that not all $m$ incidence cuts have been selected for the basis of the kernel of $L_1$ in the above proof) then the graph $G^*$ is not open, since imports have been left out from the beginning and all exports of the original system graph are unobserved and thus directed towards a new vertex now. Thus the 'basis' vectors sum up to the zero vector (cf. lemma II.4). This means that the representation of the solutions of the linear equation system by the new variables $\alpha_k$, which will be constructed below, is not unique. It is, however, easy to see that the solutions themselves as given in the theorem are unique nevertheless and equal to the solutions of an analogue equation system constructed from any $m^* + n_0 - 1$ of the 'basis' vectors, i.e. one arbitrarily selected element of $V^*$ is treated as if it were not critical. Therefore we have to take care of this special case only when the number of variables $\alpha_k$ of the mentioned equation system comes in. Finally note that $V^* = V$ is equivalent to the (rare) case where there exist only one input and one output which have the same target vertex. $\triangle$

Before drawing some conclusions from the theorem note that the weights of all cycles and paths, computed from the given solutions, are varying independently of the variables $\alpha_k$. Furthermore it is important to remark that the non-negativity constraints are incorporated in the theorem.

VI.37 Corollary

The transfer coefficients associated with elements of $E_0$ are not $\bar{\theta}_1$-identifiable. If neither the initial nor the target vertex of an edge $e_j \notin E_0$ is critical then the transfer coefficient associated with this edge is $\bar{\theta}_1$-identifiable.

Since assumption 2c gives the balance equations as additional identification equations we immediately have

VI.38 Corollary

Consider a system parameterised by $\theta_1$. Then

1. The condition $V^* = E_0 = \emptyset$ of theorem VI.36 is sufficient for $\theta_1$-identifiability.

2. If neither the initial nor the target vertex of an edge $e_j \notin E_0$ is critical then the transfer coefficient associated with this edge is $\bar{\theta}_1$-identifiable.

It is now time to drop the assumption M3$\theta_1$. Let $E_0^*$ and $n_0^*$ denote the set and the number, respectively, of edges $e_j \in E_0$ with initial vertex in $V^* \cup N^-(V^*)$ and assume that the elements of $E_0^*$ have the first indices in $E$ and thus in $E_0$. First it is important to see that the balance equation associated with a subsystem which is not in the critical set $V^*$ nor in the set $N^-(V^*)$ of its predecessors only affects edges the transfer coefficients of which are already $\theta_1$-identifiable according to corollary VI.37 or which are elements of $E_0 \setminus E_0^*$. The transfer coefficients corresponding to elements of $E_0 \setminus E_0^*$ are $\bar{\theta}_1$-identifiable (namely by the corresponding balance equations) if and only if only one such element occurs per balance equation. Since by definition $V^* = \emptyset$ implies $E_0^* = \emptyset$ the above discussion together with part 1 of corollary VI.38 results in
VI.39 Proposition
A system parameterised by \( \theta_1 \) is \( \theta_1 \)-identifiable if (i) \( V^* = \emptyset \) holds and (ii) no two elements of \( E_0 \) have the same initial vertex. The condition (ii) is necessary as well.

Proof: It remains to show that, in the case when there exist critical vertices, the second condition is necessary for \( \theta_1 \)-identifiability. For this purpose assume that a vertex \( k \in V^* \cup N^-(V^*) \) has two outflows, \( e_i \) and \( e_j \) say, which are contained in no cycle nor in any path. In view of theorem VI.36 it follows that both edges bring in a new variable \( \alpha_{m^*+j} \) which does not occur in the description of any other transfer coefficient. In addition, these variables are related only by the balance equation associated with \( k \). □

By theorem VI.36 the remaining balance equations are equations in the new variables \( \alpha_k \) \((k = 1, \ldots, m^* + n_0^*)\). The balance equation corresponding to a critical subsystem \( k \in \{1, \ldots, m^*\} \) gives an equation of the form

\[
\alpha_k^{-1} \sum_{t(e_j) \in V^*} t_j^p \alpha_{t(e_j)} + \alpha_k^{-1} \sum_{t(e_j) \not\in V^*} t_j^p + \alpha_k^{-1} \sum_{e_j \in E_0} t_j^p \alpha_{m^*+j} = 1
\]

while for subsystem \( k \in N^-(V^*) \) we have an equation of the form

\[
\sum_{t(e_j) \in V^*} t_j^p \alpha_{t(e_j)} + \sum_{t(e_j) \not\in V^*} t_j^p + \sum_{e_j \in E_0} t_j^p \alpha_{m^*+j} = 1 \tag{VI.22}
\]

where in both cases the sums are taken over edges \( e_j \) with \( s(e_j) = k \). In addition \( e_j \not\in E_0 \) is implicitly meant to hold where \( e_j \in E_0 \) is not indicated. While the latter form is already linear in the variables, the former can be transformed to be linear by multiplication with \( \alpha_k > 0 \). This gives

\[
\sum_{t(e_j) \in V^*} t_j^p \alpha_{t(e_j)} + \sum_{t(e_j) \not\in V^*} t_j^p + \sum_{e_j \in E_0} t_j^p \alpha_{m^*+j} = \alpha_k \tag{VI.23}
\]

The system (VI.22) and (VI.23) consists of \(|V^* \cup N^-(V^*)|\) linear equations in \( m^* + n_0^* \) variables.

Remark: Note that by the assumption of consistent estimates \( \hat{\Phi}^{(1)} \) and \( \hat{R}^{(1)} \) the \( t_j^p \) are such that a non-negative solution always exists. Therefore the solution is unique in the non-negative orthant if and only if it is unique in the whole vector space. Furthermore the non-negativity together with the balance equations guarantee that the solution is an element of \( P_1 \) as given in (VI.3). □

The following proposition gives a necessary condition for the uniqueness of the solution. We denote by \( n^+(k) \) the number of outflows of vertex \( k \) and assume, without restricting generality, that in the case where \( \ast \) is not fulfilled we act as if the vertex \( m \) were not critical.

VI.40 Proposition
A system parameterised by \( \theta_1 \) with \( V^* \neq \emptyset \) and satisfying condition \( \ast \) is \( \theta_1 \)-identifiable only if

\[
n_0^* \leq |N^-(V^*)| \tag{VI.24}
\]

holds. If \( \ast \) is not satisfied then (VI.24) reduces to

\[
n_0 \leq \begin{cases} 1 & \text{for } m \in N^-(V^*) \\ n^+(m) & \text{else} \end{cases}
\]
Proof: It remains to show the inequalities in the special case where the condition (9) is not satisfied, i.e. where \( V^* = V \) holds and there are no observed exports. Let \( V^* = V \setminus \{ m \} \) denote the adapted set of critical vertices such that the basis vectors (see the proof of theorem VI.36) are linearly independent. We now have to apply (VI.24) to the adapted graph.

In the case where \( m \) is not a predecessor of a critical vertex we have \( V^* \cup N^- (V^*) = V \) and thus \( n^*_0 = n_0 \). Otherwise \( n^*_0 \) equals \( n_0 \) minus the number of outflows of the vertex \( m \). □

Let us now have a closer look at the coefficient matrix, \( M \), say, of the inhomogenous linear system (VI.22) for \( k \in V^* \) and (VI.23) for \( k \in N^- (V^*) \). Assume that the rows are ordered according to the number of the subsystems to which the (transformed) balance equations correspond and that the columns are ordered according to the index of the \( \alpha_k \). Denote by \( V_i^* \) and \( N^-_i (V^*) \), \( i = 1, 2 \), the subsets of \( V^* \) and \( N^- (V^*) \), respectively, which for \( i = 2 \) contain the elements having outflows in \( E^*_0 \) (or, equivalently, in \( E_0 \)) and for \( i = 1 \) take up the remaining vertices. In addition let \( E^*_0 \) be divided into \( E^*_0 \) containing those elements \( e_j \) of \( E^*_0 \) with \( s(e_j) \in V^* \) and \( E^*_0,2 \) = \( E^*_0 \setminus E^*_0,1 \). Then, without loss of generality, \( M \) is partitioned in the following way using an obvious notation:

\[
M = \begin{pmatrix}
M_{V^*,V^*} & M_{V^*,E^*_0} \\
M_{N^- (V^*),V^*} & M_{N^- (V^*),E^*_0}
\end{pmatrix}
\]

(VI.25)

We note that there are non-zero entries in the following two cases: First, minus ones occur in the diagonal of \( M_{V^*,V^*} \). Secondly, for \( j \) with \( s(e_j) \in V^* \cup N^- (V^*) \) a particular solution \( t^*_j \) occurs in the position \((s(e_j), m^* + j)\) for \( e_j \in E^*_0 \) and in the position \((s(e_j), t(e_j))\) if \( e_j \notin E^*_0 \) and \( t(e_j) \in V^* \).

Since according to proposition VI.39 in the case of identifiability the matrices \( M_{V^*_2,E^*_0,1} \) and \( M_{N^-_2 (V^*),E^*_0,2} \) are diagonal condition (VI.24) is equivalent to

\[
m^* \leq M^* + |N^- (V^*)| \]

\[
\iff m^*_2 \leq |N^- (V^*)|,
\]

where \( m^*_i \), for \( i = 1, 2 \), is the cardinality of \( V^*_i \).

It is clear that a stronger necessary condition than the one given in proposition VI.40 is obtained by requiring the existence of a matching of the \( \alpha_k \) on the bipartite graph represented by \( M \), since each matching corresponds to one summand of the determinant of a suitable submatrix of order \( m^* + n^*_0 \). If all non-zero elements of \( M \) were varying independently this condition would also be sufficient because other summands of the determinant would have at least one different \( t^*_j \) as a factor and thus would vary independently. The following lemma will show that in our case the matching condition is also sufficient and give an alternative, graph theoretic condition.

VI.41 LEASTMA

Consider a system parameterised by \( \theta_1 \) with \( V^* \neq \emptyset \). Then the rank of the matrix

\[
\begin{pmatrix}
M_{V^*_1,V^*} \\
M_{N^- (V^*),V^*}
\end{pmatrix}
\]

(VI.26)
equals $m^* \theta_1$-generically if and only if there exists a set of vertex-disjoint paths from $N_1^-(V^*)$ to $V_2^*$ either of length one or via $V_1^*$ which cover all vertices of $V_2^*$.

Proof: First we show that each matching on the bipartite graph represented by the matrix (VI.26) corresponds to a set of vertex-disjoint paths as given in the lemma. This can be seen by starting from a column associated with an element of $V_2^*$. This is matched to a row associated with an element of $N_1^-(V_1^*)$ (then we are ready) or with an element of $V_1^*$, the column corresponding to which is again matched to a row associated with an element of $N_1^-(V_1^*)$ (then we are ready this time) or with yet another element of $V_1^*$ and so on. The remaining elements of $V_1^*$ are covered by the loops (produced by the minus ones) and eventual other cycles within $V_1^*$. In the case where $V_2^*$ is empty then the full rank as well as the existence of a matching are guaranteed by the diagonal of minus ones in $M_{V_1^*, V_2^*}$.

According to analogous arguments as in the discussion above we only have to show that the existence of a matching on the bipartite graph represented by (VI.26) is sufficient for the given matrix to have full rank. If a matching exists we may restrict our investigation of the remaining matchings to those with the same matched elements of $V_1^* \cup N_1^-(V_1^*)$, i.e. we show that the particular $m^* \times m^*$ submatrix, $S$ say, which corresponds to the rows associated with these matched elements, is non-singular.

Obviously, the true parameter values, which obey the balance equations, are contained in the manifold in $\bar{P}_1$ given by (VI.21). On the other hand the choice of the particular solutions ($\theta_{11}$ or $\theta_{12}$, for instance) within one manifold (for fixed true parameter values) has no influence on the regularity of the considered submatrix. This follows from the positivity of the $\alpha_k$ since we have

$$\det(S)_{1p, 1} = \det(S)_{1p, 2} \prod_{k \in V_2^*} \alpha_k^{1, 2}$$

where the $\alpha_k^{1, 2}$ are the values of the variables in order to shift from one particular solution to the other. Thus it suffices to show that imposing the balance equations on the particular solutions cannot lead to cancellations of the summands in the determinant to zero. This can easily be seen by expanding the determinant along any row: If the whole determinant but not all of the subdeterminants were zero then we could choose the transfer coefficients of the selected row (which are varying independently of those in the subdeterminants) so that we get away again from the zero value for the whole determinant. \square

Together with proposition VI.39 this enables us to formulate the necessary and sufficient graph theoretic condition for identifiability in the case where the balance equations are taken into account. Note that because $V_2^* \subseteq V^*$ holds we have

$$V^* = \emptyset \cup V_2^* = \emptyset \Leftrightarrow V_2^* = \emptyset$$

Since the condition (ii) of the same proposition guarantees that the matrices $M_{V_1^*, E_{1, 2}^*}$ and $M_{N_1^-(V_1^*), E_{1, 2}^*}$ are diagonal the trivial part of the matching to be found, which corresponds to these matrices, does not have to be checked for. In addition the reformulation of the matching condition as given in the above lemma is chosen. The main result of this section may thus be stated as follows:

VI.42 Theorem

For a system with $\tilde{m} = m = m_{con}$, a priori known lifetimes and parameterized by $\theta_1$ let $E_0$ denote the set of edges that are contained in no cycle and no input-output-path, $V^*$ the set of critical vertices, $V_1^*$ and $N_1^-(V_1^*)$ the subsets of $V^*$ and $N_1^-(V_1^*)$, respectively, the elements of which have no outflows in $E_0$, and set $V_2^* = V^* \setminus V_1^*$. Then the system is
\( \theta_1 \)-identifiable if and only if

(i) No two elements of \( E_0 \) have the same initial vertex

and either

(ii) \( V_2^* = \emptyset \) holds

or

(iii) There exists a set of vertex-disjoint paths from \( N_1^{-}(V^*) \) to \( V_2^* \) either of length one or via \( V_1^* \) which covers all vertices of \( V_2^* \).

We see directly from the above results that the transfer coefficient associated with an edge \( e_j \in E_0 \setminus E_0^* \) is identifiable if and only if there is no other edge in this set with the same source vertex. In addition the transfer coefficient associated with an edge \( e_j \in E_0 \) such that \( s(e_j), t(e_j) \notin V^* \) is identifiable. As another obvious consequence we have

**VI.43 Corollary**

Consider a system as described in the theorem. If \( E_0 \) is empty then the system is \( \theta_1 \)-identifiable.

**VI.44 Corollary**

If there is no a priori information in the form of known transfer coefficient equations or additional linear relations and if the system is input- and output-connectable, then it is \( \theta_1 \)-identifiable if there are no semicycles of unmeasured flows which involve the surrounding vertex.

**Proof:** First note that in the input- and output-connectable case the edges in \( E_0 \) correspond to unobserved exports or to paths of unobserved edges which lead to unobserved exports. It is then easy to see that in the case where the condition (i) of the theorem is violated the edges in \( E_0 \) form a semicycle of the required form. If, on the other hand, neither (ii) nor (iii) is satisfied then there are two cases to be distinguished: If there is an element of \( V_2^* \) which is reached within \( \tilde{G}_1(V^*) \) from an element of \( N_2^{-}(V^*) \) then again we can find such a semicycle, since all edges in \( \tilde{G}_1(V^*) \) and all edges with terminal vertex in this subgraph correspond to unmeasured flows by the definition of \( V^* \).

Thus it remains to consider the case where all elements of \( V_2^* \) can only be reached within \( \tilde{G}_1(V^*) \) from elements of \( N_1^{-}(V^*) \). Because of \( \theta_1 \)-unidentifiability we thus have a situation where there is an unmeasured path from one element of \( N_1^{-}(V^*) \) to more than one element of \( V_2^* \). This constellations, however, again forms an unmeasured semicycle involving the surrounding vertex. \( \square \)

The second corollary gives an interesting connection to the static case, since the static model in the simple case considered here is identifiable if and only if there are no semicycles of unmeasured flows (including or not including the surrounding vertex, see proposition V.7). Therefore static identifiability implies dynamic identifiability in this case.

If a considered system is not \( \theta_1 \)-identifiable according to the above conditions we may still look for indices \( k \) for which \( \alpha_k \) is uniquely determined from the equations (VI.22) and (VI.23) nevertheless. More generally, we will now investigate the exact form of the transformations between the different observationally equivalent systems. First, it is immediately clear from theorem VI.36 and from the linearity of (VI.22) and (VI.23) that in general the observationally equivalent values of a transfer coefficient \( t_j \) are given by

\[
t_j = \frac{t_j^0 a_j + b_j^0 \beta}{e_j + d_j^0 \beta}
\]
where the dimension of $\beta$ is equal to the dimension of the right kernel of $M$. If by $r$ we denote the rank of $M$, which has a graph theoretic interpretation via lemma VI.41, this dimension can be expressed as $m^* + n_0^* - r$. It remains to find out the way in which the coefficients $a_j, b_j, c_j$ and $d_j$ interact for different indices $j$.

For this purpose recall that the third condition given in theorem VI.42 is based on a matching of the $a_k, k = 1, \ldots, m^* + n_0^*$ on the bipartite graph given by the matrix $M$. In the unidentifiable case there does not exist a complete matching. However, on the basis of a maximum matching (the cardinality of which is obviously equal to the rank of $M$) we construct a graph, $G_M$ say, as follows: There exists a vertex for each element of $V^* \cup N^-(V^*)$ and for each element of $E_0^*$ (We assume that the first condition of theorem VI.42 is satisfied for all elements of $E_0 \setminus E_0^*$ since the transfer coefficients associated with the edges in this set are related only vertexwise by the balance equations). The edges between these vertices are located and weighted according to the matrix $M$. This means that the edges within $V^*$ as well as those from $N^-(V^*)$ to $V^*$ are the same as on the system graph, whereas loops with weight minus one are added to each element of $V^*$ and edges of $E_0^*$ are directed to the respective new vertex associated with it. The maximum matching is taken into account by choosing for each matched element $j$ of $V_{2}^*$ one of its successors in $G_M$ representing an $a_{m^*+}$. and linking it with the vertex in $N^-(V^*)$ with which $j$ has been matched. Each such link gets a weight equal to one. Next, for each vertex $j$ representing an element of $N_{2}^-(V^*)$ choose one of its successors in $G_M$ representing an element of $E^*_{0,2}$ and link it with $j$ with weight one. Finally add a sink, $s_M$ say, which receives an inflow from $k \in V^* \cup N^-(V^*)$ if and only if the constant term of (VI.23) or (VI.22), respectively, is different from zero. The weight of such an edge is set equal to minus the respective term.

For the formulation of the following theorem we assume that the vertices in $G_M$ corresponding to $a_{r+1}, \ldots, a_{m^*+n_0^*}$ are those which are not linked to an element of $N^-(V^*)$ according to the maximum matching. Similarly, let us assume for simplicity that the matched elements of $N^-(V^*)$ are the first $r - m^*$ ones.

**VI.45 Theorem**

Consider a system which is parameterised by $\theta_1$. Then we have

$$
\alpha_k = \begin{cases} 
\frac{\lambda_k + \mu_k \beta}{\nu} & \text{for } 1 \leq k \leq r \\
\beta_{m-r} & \text{for } r < k \leq m^* + n_0^*
\end{cases}
$$

where $\lambda_k$ is the sum of the weights of all generalised paths on $G_M$ from the vertex associated with $a_k$ to the vertex $s_M$ which cover$^9$ the first $r$ elements of $V^* \cup N^-(V^*)$, the $i$-th component of $\mu_k$ is the sum of the weights of all generalised paths on $G_M$ from the vertex associated with $a_k$ to the vertex associated with $a_{r+i}$ which cover the first $r$ elements of $V^* \cup N^-(V^*)$ and $\nu$ is the sum of the weights of all generalised cycles on $G_M$ which cover the first $r$ elements of $V^* \cup N^-(V^*)$. $\beta$ contains the parameters to describe the affine subspace of observationally equivalent values for the $\alpha_k$.

**Proof:** First note that the $\alpha_k$ are the solutions of the underdetermined system of equations given by the coefficient Matrix $M$ and the right hand side, $s$ say, which by construction is equal to the vector of the weights of the edges on $G_M$ with terminal vertex $s_M$. We choose a non-singular submatrix of $M$, $M^*$ say, according to the maximum matching which we have found during checking the condition (iii) of theorem VI.42. Therefore the columns of this submatrix correspond to $\alpha_1, \ldots, \alpha_r$, while its rows correspond to the elements of $V^*$ and $E_0^*$.

---

$^9$Note that this sum of weights is not a reduced form since the involved generalised paths may also contain the vertices corresponding to the selected successors of matched elements of $V_{2}^*$ and $N_{2}^-(V^*)$. 64
those elements of \( N^-(V^*) \) which are matched. A particular solution for the first \( r \) rows of the original equation system is then given by

\[
\begin{pmatrix}
(M^r)^{-1}s^r \\
0
\end{pmatrix}
\]

where \( s^r \) contains the first \( r \) components of \( s \). By the consistency assumption this is also a solution to the whole equation system. If we denote by \( M^d \) the first \( r \) rows of the matrix given by the columns \( r+1, \ldots, m^*+n^*_0 \) of \( M \) then the kernel of \( M \) is spanned by the columns of

\[
-(M^r)^{-1}M^d
\]

It remains to apply lemma II.8 for the inversion of \( M^r \) in order to arrive at the graph theoretic interpretation of the solutions. For this step it was necessary to identify (i.e. to link with weight one) the vertex representing \( \alpha_m + \epsilon \) on \( \mathcal{G}_M \) with the vertex representing the \( i \)-th element of \( N^-(V^*) \). \( \square \)

### VI.6.3.2 Arbitrary Lifetimes

As introduced in section VI.3 let \( \mathcal{G} \) denote the graph which emerges from the system graph \( \mathcal{G} \) by replacing each subsystem by a chain of so-called internal subsystems each of which has a lifetime equal to one and where the number of the internal subsystems is equal to the lifetime of the considered subsystem in \( \mathcal{G} \).

It is, of course, possible to check the conditions of theorem VI.42 on the extended graph \( \mathcal{G} \). We will, however, show now that the conditions of this theorem may equivalently be checked directly on the system graph:

**VI.46 Theorem**

Each of the conditions (i), (ii) and (iii) listed in theorem VI.42 is satisfied on \( \mathcal{G} \) if and only if the respective condition on \( \mathcal{G} \) is satisfied.

**Proof:** The equivalence of the respective first conditions is clear since for a chain representing a subsystem in \( \mathcal{G} \) all internal subsystems except the last one have only one outflow while the outflows of the last one correspond to those of the original subsystem in \( \mathcal{G} \). The same argumentation is also valid for the second condition.

For the condition (iii) note that a subsystem in \( \mathcal{G} \) which is an element of \( V_2^* \) corresponds to a chain of internal subsystems the last one of which lies in \( V_1^* \) while the others lie in \( V_0^* \). Thus there is a one-to-one correspondence between the paths required in the third condition for the original and for the extended graph. \( \square \)

### VI.6.4 Identifiability of the Lifetimes

Up to now, the identifiability of \( \theta_1 \)-systems has been investigated under the precondition that the lifetimes of the subsystems be known a priori. In practice, however, also the true lifetimes have to be estimated from the available data. Therefore the question arises in which cases the lifetimes of all subsystems are identifiable at all from the estimated transfer function and, if not so, the lifetimes of which subsystems can be identified separately.

Here we treat the case where it is a priori known which term in the transfer function is assigned to which generalised cycle or path.
For this purpose construct a graph $\mathcal{G}^*$ from the system graph $\mathcal{G}$ in the following way: Beside a surrounding vertex there is a vertex in $\mathcal{G}^*$ for each unmeasured flow in $\mathcal{G}$. Two such vertices are linked (with arbitrary direction) if the corresponding edges in $\mathcal{G}$ have a common terminal vertex which has an outflow not contained in $E_0$ or a common initial vertex. A vertex is linked to the surrounding vertex if the corresponding edge and a measured flow in $\mathcal{G}$ have a common terminal vertex which has an outflow not contained in $E_0$ or a common initial vertex.

The following theorem gives the answer to the first of the above posed questions. In this context we mean by an input-output path a path from the target of an input to the target of an output. In addition note that the graph consisting only of the surrounding vertex is open.

VI.47 Theorem
The lifetimes of a system parameterised by $\theta_1$ are identifiable if and only if the following conditions are satisfied:
(i) All subsystems are part of a cycle or an input-output-path and there are no common factors of the denominator and all numerators of the nominal transfer function.
(ii) There is no path of length greater than one consisting of elements of $E_0$.
(iii) The associated graph $\mathcal{G}^*$ as constructed above is open.

Proof: First, it is clear that the condition (i) is necessary. Next, consider the (directed) line graph $\mathcal{G}_L$ associated with $\mathcal{G}$. Clearly, the cycles in $\mathcal{G}_L$ correspond to the cycles in $\mathcal{G}$ while the input-output-paths in the original graph can be found in the line graph as paths from the vertex corresponding to an input to the vertex corresponding to an output. It is then easy to see that, under the first condition, the critical vertices in the line graph (gathered in $V^*_L$) are exactly the vertices corresponding to the unmeasured flows in the system graph. Let $E_{L,0}$ denote the edges of $\mathcal{G}_L$ which are not part of any cycle or path. In addition let an edge going from vertex $i$ to vertex $j$ in $\mathcal{G}_L$ be weighted by a lifetime parameter $\tau^{(i,j)}$.

All the information about the lifetimes which is contained in the estimate of the transfer function given by (VI.16) and (VI.17) are the powers of $s$ for non-zero coefficients, i.e. the sums of the lifetimes of the subsystems involved in the considered generalised cycle or path$^{10}$ in $\mathcal{G}$ or, equivalently, the sums of the weights associated with the edges involved in the corresponding generalised cycle or path in $\mathcal{G}_L$.

We may now proceed in the same way as in the proof of theorem VI.36 except that the system of equations (given by the estimated sums of lifetimes) does not have to be transformed by taking logarithms. This gives the following intermediate result:

$$
\tau^{(i,j)} = \tau^{(i,j)}(\mathcal{G}) + \begin{cases}
\gamma_j & \text{for } (i,j) \notin E_{L,0}, \ i \notin V^*_L, \ j \in V^*_L \\
-\gamma_i + \gamma_j & \text{for } (i,j) \notin E_{L,0}, \ i \in V^*_L, \ j \in V^*_L \\
-\gamma_i & \text{for } (i,j) \notin E_{L,0}, \ i \in V^*_L, \ j \notin V^*_L \\
-\gamma_i + \gamma_{m^*_L +} & \text{for } (i,j) \in E_{L,0}, \ i \in V^*_L \\
\gamma_{m^*_L +} & \text{for } (i,j) \in E_{L,0}, \ i \notin V^*_L \\
1 & \text{else}
\end{cases}
$$

(VI.27)

where $\tau^{(i,j)}(\mathcal{G})$ is a particular solution which is arbitrary for $(i,j) \in E_{L,0}$ and otherwise depends on the estimated sums of lifetimes occurring in the transfer function and where the $\gamma_k$ ($k = 1, \ldots, m^*_L + n L_0$) are the real free parameters.

$^{10}$In fact, we know the sums of the lifetimes of those subsystems which are not involved in the considered generalised cycle or path. However, we always known the sum of all lifetimes (minus $\tau^{(i,j)}$) as well.
In the same way as the balance equations were used in the preceding subsection in order to identify the free parameters we now use the fact that

$$\tau^{(i,j)} = \tau^{(k,l)}$$  \hspace{1cm} (VI.28)

holds in the cases $i = k$ or $j = l$ since for each subsystem the residence time is the same for all inflows and all outflows. If $E_{L,0}$ is empty then the basis vectors which lead to the above representation of the $\tau^{(i,j)}$ (see the proof of theorem VI.36) are the rows of the incidence matrix associated with the graph $G_{L||V^*_2}$. Thus the equations (VI.28) give, after suitable row transformations, which do not change the right kernel, an inhomogenous linear system of equations in the $\gamma_j$, the coefficient matrix of which is the transpose of the incidence matrix of the graph $G^*$. By corollary II.5 the full rank of this matrix is equivalent to the condition that $G^*$ is open.

If $E_{L,0}$ is not empty but the condition (ii) is satisfied then by condition (i) all elements of $E_0$ are exports. Thus for $e_j \in E_0$ no parameter $\gamma_j$ occurs in the equations (VI.27), but only the parameters $\gamma_{m^+_j}$, which are individual for each inflow of $s(e_j)$. However, it is obvious that the linking conditions for the construction of $G^*$ do or do not hold simultaneously for all unmeasured outflows of $s(e_j)$. Therefore the same arguments as above are applicable.

If, however, the second condition of the theorem is not fulfilled it is easy to see that the number of free parameters with index greater than $m^+_j$ cannot be reduced to zero by the equations (VI.28). $\square$

From the proof we may immediately deduce an answer to the second question posed in the beginning of this subsection:

**VI.48 Corollary**

All those parameters $\gamma_j$ in (VI.27) are uniquely determined by the equations (VI.28) which correspond to open components of $G^*$. 

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Chapter VII

A Dynamic Model with Normally Distributed Lifetime

This chapter treats the case where the pattern according to which the substance, which has entered the stock during a certain period, leaves the stock obeys restrictions taken from a discretised normal distribution (cf. [Kleijn et al. 2000]). We will see that most of the results of the previous chapter may well be applied here when some additional conditions are taken into account.

VII.1 Model Class

As in the previous chapter let \( G = (V, E) \) denote the system graph, i.e. the graph which directly corresponds to the flow sheet of the system under consideration. A discretised normal distribution will be truncated on the range \( a_j, \ldots, b_j \). These boundaries may be known a priori or estimated from flow measurement data. This means that the transfer function for this subsystem is of the form

\[
\sum_{l=a_j}^{b_j} w_l(\mu_j, \sigma_j)s^{-l}
\]

The weights \( w_l \) depend on the distribution parameters \( \mu_j \) and \( \sigma_j \) via

\[
w_l(\mu_j, \sigma_j) = \frac{f\left(\frac{l-\mu_j}{\sigma_j}\right)}{\sum_{l=a_j}^{b_j} f\left(\frac{l-\mu_j}{\sigma_j}\right)}
\]

where \( f(x) \) denotes the normal density function evaluated at \( x \).

It is important to see that this is only one possibility to discretise the continuous normal distribution on the integers. One could also imagine a discretisation via the normal distribution function or one which is only bounded from below. In addition note that in general the weights \( w_l \) are not symmetric around \( \mu_j \) (especially in the case where \( \mu_j \) is close to one of the boundaries) and that \( \mu_j \) and \( \sigma_j \) are in general not equal to the mean and the standard deviation of the resulting discrete distribution\(^1\). These parameters, however,

\(^1\)Simple Monte Carlo studies show that if \( \mu_j \) is close to \( a_j \) or \( b_j \), then it underestimates or overestimates, respectively, the mean and the standard deviation is overestimated by \( \sigma_j \).
describe the distribution uniquely. 

Subsystems with \( a_j < b_j \) will be called non-trivial. A trivial subsystem \( j \) is equivalent to a subsystem parameterised by \( \theta_1 \) with \( \tau_j = a_j = b_j \). By the length interval of a cycle (containing trivial and non-trivial subsystems) we mean the range bounded by

\[
\sum_{j \in V^s} a_j \quad \text{and} \quad \sum_{j \in V^s} b_j,
\]

where \( V^s \subseteq V \) is the set of subsystems contained in the considered cycle. For an input-output path the length interval is given by

\[
\left( \sum_{j \in V^s} a_j \right) - 1 \quad \text{and} \quad \left( \sum_{j \in V^s} b_j \right) - 1,
\]

where \( V^s \) contains all subsystems from the target of the considered input to the source of the considered output.

Figure VII.1 shows how a non-trivial subsystem with \( a_j > 1 \) can be modelled by a system of trivial subsystems. Denote by \( \tilde{G} = (\tilde{V}, \tilde{E}) \) the graph emerging from the system graph \( G \) by replacing each non-trivial subsystem by such a subgraph. Notations such as \( \tilde{V}^* \) for the critical subsystems in \( \tilde{G} \) explain themselves. By an internal subsystem of a subsystem \( j \) in \( \tilde{G} \) we mean any of the subsystems which belong to the subgraph representing \( j \) in \( \tilde{G} \). The distributor (subsystem) is the internal subsystem which receives the flows from the rest of the system. The (exact) lifetime of the distributor equals \( a_j - 1 \) while the other internal subsystems have a lifetime equal to one.

The transfer coefficients associated with the edges from the distributor to the other internal subsystems are restricted according to (VII.1). If in addition the balance equations are taken into account for all subsystems of \( \tilde{G} \) there are (under the assumption of known distribution boundaries) only two free parameters \( \mu_j, \sigma_j \) describing the stock dynamics of a non-trivial subsystem \( j \). The transfer coefficients occurring in \( \tilde{G} \) reduce to the remaining free parameters in the same way as in the previous chapter. Similarly to the definitions in section VI.3 we denote by \( \theta_2 : P_2 \rightarrow N \) the parameterisation which takes into account all these restrictions. The set \( P_2 \) of free parameters is given by, cf. (VI.3):

\[
P_2 = S_{n+1}^{-1} \times S_{n+2}^{-1} \times \ldots \times S_{n+q}^{-1} \times R^q_0 \]

where \( q \) is the number of non-trivial subsystems. The last factor corresponds to the stock parameters. By \( \tilde{\theta}_2 \) we mean the parameterisation which ignores the balance equations (including that for the distributor subsystems so that for each distributor the weight of one outflow remains free). Finally, \( \tilde{\theta}_2 \) denotes the parameterisation which attaches to each edge in \( \tilde{G} \) which is not an import an independent transfer coefficient.

Similarly to (VI.2) and the corresponding off-diagonal block described there, for each pair \((i,j)\) of vertices on the original system graph with \( i, j = 1, \ldots, m \) there is in the state transformation matrix \( \tilde{A} \) (after suitable renumbering of the subsystems of \( \tilde{G} \)) a block in the
A non-trivial subsystem with given \( a_j < b_j \) as a system of \( b_j - a_j + 2 \) trivial subsystems.

The \( i \)-th block row and the \( j \)-the block column, which for \( i = j \) has the form

\[
\begin{pmatrix}
\text{ 0  \\} & w_{b_j} & \vdots & 0 \\
& j_{b_j-a_j+1} & & \\
c & 0 & & \\
0 & & & j_{a_j-1}
\end{pmatrix}
\]

where \( 0 \) indicates a zero submatrix of appropriate dimension and \( I_{k}^{1} \) denotes a \( k \times k \) matrix with ones in the first upper diagonal. The rows and columns of the south-eastern subblock represent the chain subsystems with lifetime one which build the distributor subsystem.

For \( i \neq j \) the block has its only non-zero element at the south-west corner which gives the transfer coefficient from subsystem \( j \) to subsystem \( i \) in \( \mathcal{G} \). Note that thus by the balance equations the column sums of \( \tilde{A} \) for the first column of each block column are less than or equal to one according to whether the corresponding subsystem in \( \mathcal{G} \) has an export or not. The balance equations and the distribution restrictions guarantee that the column sums for the other columns in \( \tilde{A} \) are constantly equal to one.

For technical reasons we need the following assumptions:

**Assumption 5**

a: Each cycle in \( \mathcal{G} \) contains only one non-trivial subsystem and the length intervals of all cycles are disjoint. For each pair \((i,j)\) of an input \( e_i \) and an output \( e_j \) each path from \( t(e_i) \) to \( s(e_j) \) contains only one non-trivial subsystem and the length intervals of all paths from \( t(e_i) \) to \( s(e_j) \) are disjoint.

b: There exists at least one non-trivial subsystem in \( \mathcal{G} \) and \( a_j > 1 \) and \( b_j - a_j > 1 \) hold for each non-trivial subsystem \( j \).

c: For each non-trivial subsystem \( j \) all transfer coefficients, which are associated with the outflows of the distributor in the subgraph of \( \tilde{G} \) representing \( j \), except one\(^2\) depend on the distribution parameters \( \mu_j \) and \( a_j \) as in (VII.1).

Summing up, the parameterisation \( \theta_2 \) implicitly assumes all conditions 1, 2, 3 and 5c, whereas \( \tilde{\theta}_2 \) assumes only 1, 2a, 2b, 3 and 5c and \( \tilde{\theta}_2 \) assumes only 1, 2a, 2b and 3.

\(^2\)This exception of (any) one transfer coefficient is necessary in order not to anticipate the balance equation for the distributor.
It is important to see that the condition on the number of non-trivial subsystems per cycle and per input-output path in the assumption 5a is very restrictive. However, together with 5b, it is needed in order to reduce the identification problem for this model class to the identification problem of the model class given by $\theta_1$ or by $\tilde{\theta}_1$, respectively (note, though, that by 5b the model class discussed in the previous chapter is not contained in the one of the present chapter):

**VII.1 Proposition**

If $G$ satisfies the assumptions 5a and 5b then the graph $\tilde{G}$ associated with it as described above fulfills the assumption 4.

**VII.2 Stability**

In this section we assume that the lifetime boundaries are known a priori. By construction the state transformation matrix $\tilde{A}$ of the extended graph $\tilde{G}$ is a compartmental matrix if the balance equations are valid. Therefore the proof for the equivalence of $\theta_2$-asymptotical stability and the non-existence of traps in $\tilde{G}$ runs quite analogously to the proof of theorem VI.4. Furthermore it is clear that there exists a trap in $\tilde{G}$ exactly if there is a trap in $G$. The reason for this is the fact that the subgraphs in $\tilde{G}$ which correspond to non-trivial subsystems by construction do not contain traps.

**VII.2 Theorem**

The system structure $[\tilde{A}, \theta_2]$ is $\theta_2$-asymptotically stable if and only if $G$ contains no traps.

**VII.3 Reachability and Observability**

Also in this section we assume that the lifetime boundaries are part of the a priori knowledge. First note that the subgraphs in $\tilde{G}$ which represent non-trivial subsystems are cycle-free and that there is obviously only one possibility to cover the vertices of such a subgraph by a path from the distributor to the subsystem which has outflows to the rest of the system, cf. fig. VII.1. Therefore we have

**VII.3 Lemma**

The respective conditions $A1$, $A2$, $A1^*$ and $A2^*$ applied to $\tilde{G}$ and applied to $G$ are equivalent.

There are, however, two crucial differences to the case of the parameterisation $\theta_1$: First, the path which covers all internal subsystems of a subgraph associated with a non-trivial subsystem (see above) is not conformable with the parameterisation $\theta_2$, so that a result analogous to proposition VI.11 cannot be proved in the same manner. Secondly, $\theta_2$ is not polynomial so that the proof of theorem VI.12 cannot be directly transferred to the case of the parameterisation $\theta_2$.  

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On the other hand it is easy to see from (VII.2) that the controllability matrix (for a single input) corresponding to a subgraph representing a non-trivial subsystem is given by

\[
\begin{pmatrix}
0 & w_{a_j} & w_{a_j+1} & \cdots & w_{b_j} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\vdots & \vdots & \vdots & \ddots & w_{b_j} \\
I_{a_j-1} & 0 & \cdots & \cdots & 0
\end{pmatrix}
\]

and the observability matrix (for a single output) is given by

\[
\begin{pmatrix}
1 & 0 & \cdots & 0 & 0 & \cdots & \cdots & 0 \\
0 & \ddots & \cdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & 0 \\
0 & \cdots & 1 & \cdots & \vdots & \vdots & \ddots & \vdots \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
0 & \cdots & \cdots & \cdots & \vdots & \vdots & \ddots & \vdots \\
0 & \cdots & \cdots & \cdots & \cdots & \vdots & 0 & w_{a_j} \\
0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & w_{b_j}
\end{pmatrix}
\]

where the left block column contains \( b_j - a_j + 1 \) columns.

This shows that unreachability and unobservability occur only in the degenerate case of \( \sigma_j = \infty \). In simple cases this might help to check reachability and observability. In general, however, we can only give the following simple necessary condition, which follows from corollary VI.13 and the lemma above:

**VII.4 Proposition**

If the system structure \([\bar{A}, \bar{B}, \theta_2]\) is \( \theta_2\)-reachable then the conditions A1 and A2 are fulfilled on the original system graph \( \mathcal{G} \).

**VII.4 Identifiability**

In view of proposition VII.1 we assume conditions 5a and 5b for this section.

**VII.4.1 Graph Theoretic Conditions with Known Lifetime Boundaries**

Obviously a non-trivial subsystem in \( \mathcal{G} \) is critical if and only if the corresponding distributor subsystem is critical in \( \bar{\mathcal{G}} \). By the existence of non-trivial subsystems \( \bar{\mathcal{V}}^\infty \) is not empty since all internal subsystems (except, possibly, the distributor subsystems) are critical. This gives the following proposition as a direct consequence of theorem VI.36 and proposition VII.1.
VII.5 Proposition
A system parameterised by $\tilde{\theta}_1$ is not $\tilde{\theta}_2$-identifiable. The solutions of the identification equations for the transfer coefficients $\tilde{t}_j$ in $\tilde{G}$ are given as

$$\tilde{t}_j = \tilde{P}_j^*, \quad \begin{cases} 
\tilde{a}_{l(e_j)} & \text{for } e_j \notin \tilde{E}_0, \ s(e_j) \notin \tilde{V}^*, \ t(e_j) \in \tilde{V}^* \\
\tilde{a}_{l(e_j)}^{-1} \tilde{a}_{l(e_j)} & \text{for } e_j \notin \tilde{E}_0, \ s(e_j) \in \tilde{V}^*, \ t(e_j) \in \tilde{V}^* \\
\tilde{a}_{l(e_j)}^{-1} \tilde{a}_{l(e_j)} & \text{for } e_j \notin \tilde{E}_0, \ s(e_j) \in \tilde{V}^*, \ t(e_j) \notin \tilde{V}^* \\
\tilde{a}_{l(e_j)}^{-1} \tilde{a}_{m^{**}} & \text{for } e_j \in \tilde{E}_0, \ s(e_j) \in \tilde{V}^* \\
\tilde{a}_{m^{**}} & \text{for } e_j \in \tilde{E}_0, \ s(e_j) \notin \tilde{V}^* \\
1 & \text{else} 
\end{cases}$$

where $\tilde{P}_j^*$ is a positive particular solution which is arbitrary for $e_j \in \tilde{E}_0$ and otherwise depends on the $\tilde{\theta}_1^{[1]}$ and $\tilde{R}_1^{[1]}$, and where the $\tilde{a}_{ki}$ ($k = 1, \ldots, \tilde{m}^* + \tilde{n}_0$) are the positive real free parameters.

Let us now introduce a renumbering of the subsystems in $\tilde{G}$ by index pairs: for $j > 0$ the pair $(j,k)$ denotes the $j$-th internal subsystem of the $j$-th $\theta_k$-subsystem in $G$, where (for simplicity) the distributor subsystem gets the index $(j,a_j - 1)$, the (internal) subsystem with outputs to the rest of the system gets $(j,a_j)$, its predecessor different from the distributor gets $(j,a_j + 1)$ and so on so that the (internal) subsystem giving the longest path through $j$ has number $(j,b_j)$. The index pair $(0,j)$, finally, corresponds to a trivial subsystem $j$.

Since the distribution restrictions involve the outflows of only one (internal) subsystem each (namely the distributor), they can be applied independently from each other. For fixed $j$ (in order to keep the notation simple), denote by $\tilde{t}_k, k = a_j, \ldots, b_j$ the transfer coefficients associated with the edges from the distributor subsystem to the internal subsystem $(j,k)$, see fig. VII.2.

VII.6 Proposition
Consider a system parameterised by $\tilde{\theta}_2$ and let all non-trivial subsystems be part of a cycle or a path. Then for all $j > 0$ the variables $\tilde{a}_{j,k}$ depend on each other in the following manner:

$$\tilde{a}_{j,k} = \tilde{a}_{j,k}^p (\mu_j, \sigma_j^2) \beta_j, \quad \forall k = a_j, \ldots, b_j, \quad (VII.3)$$

where $\beta_j$ is positive and a set of positive particular solutions $\tilde{a}_{j,k}^p (\mu_j, \sigma_j^2)$ is given by

$$\tilde{a}_{j,a_j+l}^p (\mu_j, \sigma_j^2) = \begin{cases} 
\frac{\sigma_j^{a_j+l+1}}{\sigma_j^{a_j+l}} \exp \left((-1)^{l/2} \frac{a_j+l+1/2}{\sigma_j^2}\right) & \text{for even } l, 0 \leq l \leq b_j - a_j \\
1 & \text{for odd } l, 0 \leq l \leq b_j - a_j 
\end{cases}$$

Proof: Consider a fixed non-trivial subsystem $j > 0$ in $G$. From section VII.1 we know that the distribution restrictions are given as

$$\log(\tilde{t}_k) - \log(\tilde{t}_{k+1}) = \frac{k - \mu_j + 1/2}{\sigma_j^2} \quad \forall k = a_j, \ldots, b_j - 1$$

By proposition VII.5 and after changing to the alternative numbering of subsystems this gives for all $k = a_j, \ldots, b_j - 1$

$$\log(\tilde{P}_k^*) - \log(\tilde{a}_{j,a_j-1}) + \log(\tilde{a}_{j,k}) - \log(\tilde{P}_{k+1}) + \log(\tilde{a}_{j,a_j-1}) - \log(\tilde{a}_{j,k+1}) = \frac{k - \mu_j + 1/2}{\sigma_j^2}$$

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if the distributor subsystem is critical and
\[
\log(\tilde{P}_k^P) + \log(\tilde{\alpha}_{j,k}) - \log(\tilde{P}_{k+1}^P) - \log(\tilde{\alpha}_{j,k+1}) = \frac{k - \mu_j + 1/2}{\sigma_j^2}
\]
if it is not. In any case these equations form a linear system of equations in the variables \(\log(\tilde{\alpha}_{j,k})\), \(k = a_j, \ldots, b_j\) with the \((b_j - a_j) \times (b_j - a_j + 1)\) coefficient matrix
\[
\begin{pmatrix}
1 & -1 \\
1 & -1 \\
& & \ddots & & \ddots \\
& & & 1 & -1
\end{pmatrix}
\]
Since its kernel is spanned by \((1, \ldots, 1)'\) taking the exponential of the solution for each variable finishes the proof. \(\square\)

The following theorem shows that, if the non-trivial subsystems are located according to \(M_{\theta_j}\), the identifiability conditions as given in theorem VI.42 remain valid and need to be checked only on the original system graph \(\mathcal{G}\).

**VII.7 Theorem**

A system parameterised by \(\theta_2\) is \(\theta_2\)-identifiable if and only if the following two conditions:

(i) No two elements of \(E_0\) have the same initial vertex.

(ii) Each non-trivial subsystem is part of a cycle or a path in \(\mathcal{G}\).

and one of the following conditions is satisfied:

(iii) \(V_\ast^2 = 0\) holds.

(iv) There exists a set of vertex-disjoint paths in \(\mathcal{G}\) from \(N^{-1}(V^\ast)\) to \(V_\ast^2\) either of length one or via \(V_\ast^2\) which covers all vertices of \(V_\ast^2\).

**Proof:** The main task is to show that, from the viewpoint of identifiability checking, non-trivial subsystems can be treated in the same manner as \(\theta_1\)-subsystems, i.e. it suffices to look at the original system graph \(\mathcal{G}\).

For this purpose consider a fixed non-trivial subsystem \(j > 0\) and the balance equation for an internal subsystem \((j, k)\) with \(k \in \{a_j + 1, \ldots, b_j - 1\}\), where, for simplicity of notation, we assume here for fixed \(j\) that \(\tilde{t}_{b_j + k}\) is the transfer coefficient corresponding to the edge from subsystem \((j, k)\) to subsystem \((j, k - 1)\), see fig. VII.2:
\[
\tilde{t}_{b_j + k}^{-1} \tilde{\alpha}_{j,k-1} = 1
\]

By proposition VII.6 and after taking logarithms this gives for each \(k - a_j\):
\[
\log(\tilde{P}_{b_j+k}^P / \tilde{P}_{k+1}^P) + (-1)^{(k-a_j)/2+1} \frac{k - \mu_j + 1/2}{\sigma_j^2} = 0
\]

The predecessor subsystem \((j, k + 1)\) analogously yields the equation
\[
\log(\tilde{P}_{b_j+k+1}^P / \tilde{P}_{k+1}^P) + (-1)^{(k-a_j)/2} \frac{k - \mu_j + 1/2}{\sigma_j^2} = 0
\]

Thus we obtain a system of two linear equations in \(\mu_j\) and \(\sigma_j^2\) where the determinant of the coefficient matrix equals
\[
(-1)^{(k-a_j)/2} \left( \log(\tilde{P}_{b_j+k+1}^P / \tilde{P}_{k+1}^P) + \log(\tilde{P}_{b_j+k}^P / \tilde{P}_{k+1}^P) \right)
\]

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which reduces to

$$\pm \log (\beta^0_{j,k+1} \beta^0_{j,k})$$

Since the two involved particular solutions, without loss of generality, are not reciprocal to one another the equation system has a unique solution. Note that by the usual consistency argument we may assume that a non-negative solution always exists and, furthermore, that the other balance equations for subsystems \((j,k)\) with \(k \in \{a_j+1, \ldots, b_j-1\}\) bring in no new information. Thus we obtain unique values for the particular solutions \(\alpha^0_{j,k}, k = a_j, \ldots, b_j\). When we now take into account the remaining balance equations, namely those for the distributor subsystem\(^3\), for the subsystem \((j,a_j)\) and for the rest of the system, we have to distinguish two cases:

If the distributor subsystem is not critical in \(\bar{G}\) the associated balance equation leads to

$$\beta_j \sum_{k=a_j}^{b_j} \beta^0_k \alpha^0_{j,k} = 1$$

which yields a unique solution for \(\beta_j\) and thus for all \(\alpha_{j,k}, k = a_j, \ldots, b_j\). This means that all internal subsystems may be taken as uncritical which is in full accordance with the fact that in this case the considered non-trivial subsystem \(j\) is uncritical in \(G\).

If on the other hand \((j,a_j-1) \in \Gamma^*\) holds then the associated balance equation gives

$$\beta_j \sum_{k=a_j}^{b_j} \beta^0_k \alpha^0_{j,k} = \alpha_{j,a_j-1} \quad \text{(VII.4)}$$

Together with (VII.3) for \(k = a_j\) we obtain a linear relation between the variables corresponding to the distributor subsystem and to the subsystem with outflows to the rest of the system:

$$\alpha_{j,a_j-1} = \left( (\alpha^0_{j,a_j})^{-1} \sum_{k=a_j}^{b_j} \beta^0_k \alpha^0_{j,k} \right) \alpha_{j,a_j} \quad \text{(VII.5)}$$

This equation, however, has very much the same form as (VI.23), i.e. in the procedure of subsection VI.6.3 leading to theorem VI.42 it plays the roll of the balance equation for the

\(^{3}\text{Note that the balance equation for the distributor subsystem in fact is a distribution restriction which, however, has not yet been taken as such according to condition M4.}\)
distributor with a special particular solution. Therefore, and since \( \alpha_{j,k}, k = a_j + 1, \ldots, b_j \) are determined (by (VII.4) or (VII.5), respectively, and (VII.3)) as soon as \( \alpha_{j,a_j-1} \) or \( \alpha_{j,a_j} \) is determined, we may reduce the inner structure of the considered non-trivial subsystem to the subsystems \((j, a_j - 1)\) and \((j, a_j)\) which are linked by an edge with associated particular solution as given in (VII.5). Denote the resulting graph by \( \mathcal{G} = (V, E) \). While the distributor is obviously an element of \( V \), because of condition (ii) and since the edge going to \((j, a_j)\) is the only outflow, \((j, a_j)\) may be in the same set or in \( V^* \). In the first case the graph theoretic conditions of theorem VI.42 are trivially the same when applied to \( \mathcal{G} \) and to \( \mathcal{G} \). In the second case the same is true since then the whole non-trivial subsystem is an element of \( V^* \). In any case the balance equation associated with \((j, a_j)\) in \( \mathcal{G} \) corresponds to the balance equation of the whole subsystem \( j \) in \( \mathcal{G} \). Hence the proof that it suffices to investigate the original system graph \( \mathcal{G} \) is complete if lemma VI.41 applied to \( \mathcal{G} \) is also valid when the special particular solution occurring in (VII.5) is one of the non-zero elements of the matrix \( M_{V^*_1, V^*_2} \). This, however, is true since the expression in brackets in (VII.5) only depends on internal \( \mathcal{P} \).

The following considerations immediately finish the proof of the theorem: If a non-trivial subsystem is not part of any cycle nor of any path then considerations analogous to those in proposition VII.6 lead to a dependence not between the variables associated with the internal subsystems but between the variables associated with the edges away from the distributor subsystem, which are elements of \( E_0 \). It is obvious that the balance equations corresponding to the internal subsystems cannot relate these variables. Thus we have unidentifiability. If, on the other hand, condition (ii) is fulfilled then condition (i) together with (iii) or (iv) are equivalent to identifiability in the same way as in the case of no non-trivial subsystems. \( \square \)

### VII.4.2 Identifiability of the Lifetime Boundaries

Basically, the problem of identifiability of the \( a_j \) and \( b_j \) for all non-trivial subsystems and of the \( \tau_j = a_j = b_j \) for all trivial subsystems is the same as in the case of the parameterisation \( \theta_1 \), since an overlapping of length intervals within generalised cycles or paths is precluded by assumption 5a. The only difference is that in addition to separate terms with a power of \( s \) equal to some \( \sum_{i \in V'} \tau_i \), there also occur successive terms with powers ranging from

\[
a_j + \sum_{i \in V'} \tau_i \quad \text{to} \quad b_j + \sum_{i \in V'} \tau_i
\]

Thus, as long as the terms corresponding to these ranges as well as the separate terms are a priori assigned to specific generalised cycles and paths, the powers of the separate terms and the bounds of the ranges for each non-trivial subsystem enter the identification equations which lead to (VI.27).
CHAPTER VIII

A DYNAMIC MODEL WITH
GEOMETRICALLY DECLINING
LIFETIME

The second example for the applicability of the results proved for the case with exact lifetime on cases with more complex stock behaviour deals with a geometrically declining lifetime pattern. This case is certainly more relevant in the description of natural stocks, i.e. stocks which are left to the geo-physical influences, than of economic stocks. Furthermore it is a good example to show which additional possibilities, but also which additional problems are created by releasing one of the basic assumptions implicitly underlying the prototype parameterisation $\theta_1$.

VIII.1 Model Class

Let $\mathcal{G}$ again denote the system graph which directly corresponds to the underlying flow sheet. The motivation for the stock behaviour we treat in this chapter is the following: Assume that the (single) outflow, $y_{i,t}$ say, of the stock of the $j$-th subsystem is equal to a certain portion of the level of this stock, denoted by $x_{j,t}$ so that

$$y_{i,t} = \kappa_j x_{j,t}$$

holds. This portion $\kappa_j \in [0,1)$ will be considered constant over time but generally unknown a priori so that it has to be estimated from the flow data. This results in a transfer function for the $j$-th subsystem of the form

$$\sum_{i=1}^{\infty} \kappa_j (1 - \kappa_j)^{i-1} s^{-i}$$

Subsystems with such a transfer function will be called non-trivial in this chapter, while those with exact lifetime will be said to be trivial. By excluding the value one for $\kappa_j$ we assume that it is a priori known which subsystems are trivial and which are non-trivial. Now it is immediately obvious that this declining pattern can be modeled by a dynamic subsystem with exact lifetime equal to one and a loop with weight $1 - \kappa_j$. To be more precise, a subsystem with geometrically declining lifetime depending on a parameter $\kappa_j$ and outflows
A Dynamic Model with Geometrically Declining Lifetime

VIII.1 Model Class

Figure VIII.1: A non-trivial subsystem in \( \mathcal{G} \) (left, with parameter \( \kappa_j \)) and its representation in \( \hat{\mathcal{G}} \) (right).

with transfer coefficients \( t_{j_1}, \ldots, t_{j_h} \) is represented in an extended graph \( \hat{\mathcal{G}} = (\hat{V}, \hat{E}) \) as a subsystem with exact lifetime. It is reasonable to assume that the (artificial) flow associated with the loop is not measured and that, in analogy with assumption 1b, there is at most one loop per subsystem in \( \hat{\mathcal{G}} \). It is important to note that, unlike the extended graphs in the preceding chapter and in the subsection VI.6.3.2, here we have \( \hat{\mathcal{V}} = \mathcal{V} \).

Let the weight of the loop be denoted by \( \tilde{t}_{j_h} \) and the weights for the remaining outflows by \( \tilde{t}_{j_{h-1}}, \ldots, \tilde{t}_{j_1} \). Then there is for each non-trivial subsystem \( j \) a bijective correspondence between the transfer coefficients and the dynamic parameter in the system represented by \( \mathcal{G} \) on the one hand and the transfer coefficients in the system represented by \( \hat{\mathcal{G}} \) on the other hand, see also fig. VIII.1.

\[
\begin{align*}
1 - \kappa_j & \leftrightarrow \tilde{t}_{j_h} \\
\kappa_j t_{j_1} & \leftrightarrow \tilde{t}_{j_{h-1}} \\
\vdots & \\
\kappa_j t_{j_h} & \leftrightarrow \tilde{t}_{j_1} 
\end{align*}
\]

The parameterisation, \( \theta_0 \) say, suitable for the description of a system containing such non-trivial subsystems is identical with the parameterisation \( \theta_1 \) for the system associated with the extended system graph \( \hat{\mathcal{G}} \). Analogously, \( \theta_2 \) is identical with \( \theta_1 \) for this extended system. Note, however, that the assumption 1c, which refers to the original system graph \( \mathcal{G} \), is implicitly assumed for both \( \theta_2 \) and \( \theta_3 \).

Clearly, the structure of the system matrices corresponding to a system parameterised by \( \theta_3 \) differs from that described in section VI.3 only in the fact that those diagonal blocks which represent non-trivial subsystems are \( 1 \times 1 \) matrices with a non-zero entry.

The following assumption will be needed in order to be able to use the results for \( \theta_1 \) in this case.

Assumption 6

The length\(^1\) of the smallest cycle which is not a loop is greater than the number of non-trivial subsystems.

It is not clear how restrictive this condition is in practical applications: On the one hand it can be expected that the number of non-trivial subsystems with geometrically declining behaviour is rather small. On the other hand assumption 6 is easily violated if there are cycles involving only a few subsystems a great part of which are non-trivial.

\(^1\)Counted as the sum of the (exact) lifetimes of the involved subsystems. Recall that a non-trivial subsystem is modelled with exact lifetime equal to one.

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VIII.2 Stability

A generic zero value for $\kappa_j$ means that the non-trivial subsystem $j$ alone is a trap in $\tilde{\mathcal{G}}$. This case, however, implies that $j$ has no outflows in $\mathcal{G}$ and is thus also a trap in $\mathcal{G}$. The other constellations of traps are the same in $\tilde{\mathcal{G}}$ and in $\mathcal{G}$. Therefore, following the same arguments as in the preceding chapter, we may directly conclude from theorem VI.4:

VIII.1 Theorem
The system structure $[A, \theta_3]$ is $\theta_3$-asymptotically stable if and only if $\mathcal{G}$ contains no traps.

VIII.3 Reachability and Observability

Prohibiting loops for the parameterisation $\theta_1$ mainly had practical reasons, namely that we did not think them to be useful in the context of material flow systems. However, the corresponding assumption 1c was technically needed only in the investigation of identifiability. Therefore we may directly transfer the results on $\theta_1$-reachability and $\theta_1$-observability to the parameterisation $\theta_3$ with only a small modification of the conditions A2 and A2* which is due to the fact that the vertices in $\tilde{\mathcal{G}}$ with loops are automatically covered by cycles. The modified conditions are given as:

A2*: On the system graph $\mathcal{G}$ there exists a family of disjoint cycles and stems such that all vertices associated with trivial subsystems are covered.

A2**: On the system graph $\mathcal{G}$ there exists a family of disjoint cycles and output stems such that all vertices associated with trivial subsystems are covered.

This leads to:

VIII.2 Theorem
1. $[A, B, \theta_3]$ is $\theta_3$-reachable if and only if the conditions A1 and A2* are both satisfied.
2. $[A, C, \theta_3]$ is $\theta_3$-observable if and only if the conditions A1* and A2** are both satisfied.

VIII.4 Identifiability

We will also in the investigation of identifiability try to use the results deduced for the case of exact lifetimes. For this purpose we assume that the condition 4, which refers to the original system graph $\mathcal{G}$, as well as the condition 6 are valid. Under these assumptions we will give necessary and sufficient conditions for local identifiability which is defined as follows:

Definition: A system of a given model class is $\theta$-generically locally identifiable if for all choices of the free parameters except on an algebraic set there exists a neighbourhood such that the function, which maps the non-negative free parameters on the space of transfer functions, restricted to this neighbourhood is injective.

Remark: Note that the edges building loops in $\tilde{\mathcal{G}}$ never are elements of $\tilde{E}_0$. Thus the first condition in the definition of a critical vertex, which requires an edge not in $E_0$ or $E_0$, respectively, incident to it, is always fulfilled in $\tilde{\mathcal{G}}$ for non-trivial subsystems. As a consequence $\mathcal{V}^* \neq \tilde{\mathcal{V}}^*$ holds in general. Of course, we like to give conditions referring to the original system graph $\mathcal{G}$, although the graph which is crucial for the identifiability...
conditions to be found is $\tilde{G}$. However, it will not cause any confusion if our conditions refer to $\tilde{V}^*$ when we keep in mind that $k \in \tilde{V}^*$ holds if and only if $k$ is critical in $G$ or if it is non-trivial and satisfies the second condition of lemma VI.35. $<$

In the case of geometrically declining stock patterns the identification equations analogous to (VI.20) contain also the transfer coefficients associated with the loops in $\tilde{G}$. In the following we will first solve those equations which contain only these transfer coefficients. Under assumption 6 this leads to finitely many solutions, for each of which we may then solve the remaining system of equations in the same way as for the parameterisation $\theta_1$. Let $m_n$ denote the number of non-trivial subsystems.

**VIII.3 Proposition**

Under assumption 6 there are $m_n$ identification equations which contain only transfer coefficients associated with the loops in $\tilde{G}$. These equations have exactly $m_n!$ solutions. Each of the solutions emerges from the other by a permutation of components.

**Proof:** For simplicity of notation let $a_j$ denote the transfer coefficient associated with the loop of the $j$-th non-trivial subsystem. By assumption the identification equations corresponding to the generalised cycles of length $1, 2, \ldots, m_n$ have the following form:

\[
a_1 + a_2 + \cdots + a_{m_n} = \varphi^{(1)}_{\tilde{V}}
\]

\[
a_1 a_2 + a_1 a_3 + \cdots + a_1 a_{m_n} + a_2 a_3 + \cdots + a_{m_n-1} a_{m_n} = \varphi^{(2)}_{\tilde{V}}
\]

\[
\vdots
\]

\[
a_1 a_2 \cdots a_{m_n} = \varphi^{(m_n)}_{\tilde{V}}
\]

It is easy to see that by sequential substitution this equation system leads to the single equation

\[
(a_1)^{m_n} + \sum_{i=1}^{m_n} (-1)^i \varphi^{(i)}_{\tilde{V}} (a_1)^{m_n-i} = 0
\]

(VIII.2)

The second statement in the proposition is trivially true for $m_n = 1$. Assume that it has also been shown for $m_n - 1$. Let $\bar{a}$ denote any of the $m_n$ solutions of (VIII.2). Then dividing this equation by $(a_1 - \bar{a})$ gives

\[
(a_1)^{m_n-1} + \sum_{i=1}^{m_n-1} (-1)^i \varphi^{(i)}_{\tilde{V} \setminus \{m_n\}} (a_1)^{m_n-i} = 0
\]

The connection of the solutions by permutation of the components is clear since the equations (VIII.1) are symmetric in the $a_j, j = 1, \ldots, m_n$. $\square$

Since by the assumption of consistent right-hand sides of the identification equations there exists a non-negative solution so that, by the proposition, all solutions for the loop transfer coefficients have to be non-negative.

**VIII.4 Theorem**

A system parameterised by $\theta_3$ is $\theta_3$-generically locally identifiable if and only if

(i) No two elements of $E_0$ have the same initial vertex

and either
(ii) $V_2^* = \emptyset$ holds

or

(iii) There exists a set of vertex-disjoint paths from $N_1^-(V^*)$ to $V_2^*$ either of length one or via $V_1^*$ which covers all vertices of $V_2^*$.

Proof: For any of the finitely many solutions for the loop transfer coefficients as shown above we can reduce the remaining identification equations analogously to proposition VI.33 such that we have an equation for each cycle and for each input-output path on $G$. Applying theorem VI.42 gives the stated results. □

It has to be stressed that the procedure proposed here is not the most we can get for concrete systems, since a simultaneous solution of all identification equations - under assumption 6 or not - might restrict the number of solutions and even yield global identifiability.
CHAPTER IX

CONCLUSIONS AND FINAL REMARKS

When I started to work on mathematical models for material flow systems together with my colleagues in 1996 it was not at all clear which aspect of this topic would mainly attract my interest. However, already during the elaboration of the static model it became obvious that the representation of such systems by a flow sheet and thus by a directed (system) graph could yield the link between the language of system theory and that of Material Flow Analysis. This means that system theoretic questions, which occur in advance of practical problems such as parameter estimation or prediction from flow measurement data, can be formulated and solved with the help of graph theoretic concepts and methods. Thus the conditions for, e.g., stability are finally given as conditions on the system graph such that an interpretation in terms of MFA often suggests itself. Further encouraged by the cited articles on reachability and identifiability of compartmental systems, I started to deal with elementary graph theory. Soon the question was, how far I could get on this way. Quite often, as for instance in the formulation of the first dynamic model class, it was necessary to narrow the path in order to be able to go on on the basis of a graph theoretic interpretation of the transfer function. However, it is clear that the question of balance between the width and the depth in the allocation of our interests and our energy is not only a difficult and at the same time a crucial one in all fields of research but also in our personal lives.

The treatment of the static model in chapter V is to a certain extent complete except for policy simulation which was not included in this work. In [Gleiß et al., 1998] the applicability of this model (including policy simulations) has been proved. However, we experienced that two of the central assumptions of our model sometimes are problematic from a practical point of view, namely linearity and normality. Certain natural processes simply do not show a linear dependence of the outputs upon the inputs. One example, which occurred in the case study treated in the paper cited above, is the erosion of phosphorous from agricultural soils. The normal distribution of the measurements, which implies positivity and symmetry, is often reported to be inadequate. However, on the one hand the approximation based on our assumptions will be sufficient in many cases. On the other hand the extensive theory available for the linear case (under normality) allows for the development of a rather self-contained model together with practically relevant tools such as origins analysis. Furthermore there are of course still aspects in our static model
which have not been treated here, as for example the detection of gross errors (relevant literature is given in the beginning of section V.4).

In the dynamic case the catalogue of assumptions on which the investigations in this thesis are based is even larger (see section VI.1 and the model class section in chapters VI to VIII). While some of these seem to be quite natural, such as the condition that the system graph is a connected open graph, others probably do restrict the practical applicability of the model. Unlike the static model, the dynamic one has not been applied yet to practical material flow problems.

Just in order to mention some of the shortcomings, the requirement that the (system theoretic) inputs coincide with the imports into the whole system is violated as soon as an internal flow, such as consumer’s demand for certain goods, is driving the system. While loosening this assumption would probably call for quite a different approach (in particular if the inputs are observed with noise), the condition of the absence of parallel flows will only lead to some special cases to be considered in the proofs.

Beside presenting more flexible patterns of stock dynamics it was the purpose of the two preceding chapters to investigate how robust the results achieved for the prototype (with exact lifetimes) are against adding restrictions or relaxing one or the other existing assumption, respectively. E.g., allowing for loops on the system graph made it necessary to weaken the identifiability results from global to local identifiability. A question of interest in this context is, of course, whether other stock patterns, such as a Poisson type, can as well be treated in a similar manner, namely within a generalisation of the simple first model class. Another challenge could be the reachability or identifiability of a system which consists of subsystems of different stock types. It should not be too difficult to combine the three types introduced in this work in one model, if the different additional assumptions are taken care of.

Despite all the scepticism filling the last few paragraphs, it is worth mentioning that the results received in this thesis are of some importance. First, the discrete-time case, which due to practical reasons is mostly not dealt with in the context of compartmental systems, has been treated here. The relevance of this difference can, for example, be seen in subsection VI.5.1: The graph theoretic interpretation of the lemma by Corfmat and Morse for the continuous-time case by Hayakawa and his co-workers runs quite different to that presented here. The same section also investigates reachability conditions which originally have been proved for the case where all non-zero elements of the system matrices are varying independently of each other. Section VI.6.3 on identifiability tries to fill at least a part of a gap in compartmental modelling which has already been complained about by the pioneers of this branch of research and could, to the author’s knowledge, up to now be treated satisfactorily only for very particular cases. We are talking about general necessary and sufficient graph theoretic conditions for global identifiability. Although still some technical restrictions have been necessary, the resulting model class is of some generality: In the case of arbitrary (but exactly known) lifetimes, i.e. lifetimes greater than one, cycles or input-output paths of the same length will not be the general case.

What has to be the next step clearly is the development of efficient estimation procedures. Approaches in this direction can be found, e.g., in [Dasgupta et al., 1988], [Almasy, 1990] and [Darquier and Zasadzinski, 1991], see [Van Den Hof, 1998] for conditions for persistence of excitation. One difficulty of this task is the lack of data available for testing possible methods. Time series of flow measurements over periods would be needed which are longer than the lifetimes of the stocks in the system. The estimation not only of the transfer coefficients and the stock parameters but also of the lifetimes will require corresponding
methods. In the same way as the results obtained for compartmental models in the cited literature could only be used here under restrictions (see also chapter IV), it is not clear inasmuch the results of this work are of use in compartmental analysis in general. Since, however, environmental science in general and Material Flow Analysis in particular will even gain greater relevance in the near future due to the progressive occupation of the environment by human activities, the efforts invested into this work would be justified if the results could be of use in this field only.
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