Process Network Optimality

by

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A DISSERTATION
SUBMITTED TO THE GRADUATE SCHOOL
IN PARTIAL FULFILLMENT OF THE REQUIREMENTS

for the degree of

DOCTOR OF PHILOSOPHY
in
CHEMICAL ENGINEERING

Carnegie Institute of Technology
Department of Chemical Engineering
Carnegie Mellon University
Pittsburgh, Pennsylvania, USA

April 2010

Abstract

A novel framework is developed for the modeling and analysis of complex process networks. Interconnections among process network units are represented through connectivity matrices and network graphs. We derive a potential function based on the content and cocontent of the process network using Tellegen's theorem. This potential function, which is equivalent to the non-equilibrium entropy production in a steady state steady system, serves as a starting point to show how process networks can be regarded as gradient systems. Further, we apply the theory to derive the Euler-Lagrange equations which define the dynamic trajectory of the process network. The theory we develop can be used in many application domains including design of plant-wide decentralized control systems, decentralized optimization, stability analysis of hybrid systems, and asynchronous dynamic simulation. The basic requirement is that the flow conditions can be expressed in terms of conic sector (passivity) conditions. We illustrate how distributed control and optimization can be implemented into process network structures and how optimality conditions can be shaped through control laws and algorithms.

Tellegen's theorem as a topological invariant of the system plays a central role in physical flow networks, since it represents a power balance. We demonstrate how Tellegen's theorem can be used as a redundant constraint to assist in strengthening relaxations of process network models used in global optimization.

The theory is applied to flow of liquids in porous rock as commonly found in petroleum reservoirs. A reservoir model's grid cells are regarded as process nodes, and the production wells as network terminals. Flow is induced through potential gradients between the grid cells. We derive a potential function for the reservoir pressure and water-oil distribution for the water flooding process. This potential function, which is based on the entropy production, allows us to describe the reservoir as a gradient system such that the state trajectories minimize the energy dissipation for a given set of boundary and initial conditions. Several examples illustrate how these results affect decision-making during the displacement process for the optimization of the oil recovery process.

Acknowledgments

First, I would like to thank Bruce, Ignacio, Nick, and Erik for being on my committee, the Department of Chemical Engineering, and ultimately the entire Carnegie Mellon University community. My PhD was a unique learning experience in a very creative and stimulating environment and I have been trying my best to return some of what has been invested into me during those years through my work. However, it will probably take me a lifetime -at least- to return this debt. I am also especially thankful to Bjarne Foss from NTNU for the financial and intellectual support and to Jan Dirk Jansen from TU Delft for teaching me about reservoir engineering and our discussions of my work. I gratefully acknowledge funding from the Center of Integrated Operations in the Petroleum Industry at NTNU, Trondheim, Norway. Finally, I would like to thank my wife Mangala, my German and Indian family, my friends, and most of all you, Erik, for whom I wrote this poem.

Process Network Optimality

Process Network Optimality
an outburst of irrationality?
A student-teacher duality?
Or a glimpse of geniality?

It began in mid twothousandsix,
when Erik explained to my surprise,
that basic laws of thermodynamics
describe an *adaptive enterprise*[1].

[1]For more information, see "Distributed decision making in complex organizations: The adaptive enterprise.", B.E. Ydstie, Comp. and Chem. Eng., 2004

The daunting question which Erik had asked
was: What is a *networks'* objective?
It made me feel as having been tasked
to be a *process control* detective!

The initial road to find the solution,
led me to *Tellegen's* methodology.
"Incidentally" a *matrix* revolution,
allowed integration of *topology*.

The *objective functions*, I gladly disclosed,
are *Legendre transforms* of one another.
As *content* and *cocontent* functions exposed,
holding their *dual* "twin-hands" like brother and brother.

The network work was fairly revealing,
and "qualified" me for further studies.
The Norwegians found the work quite appealing,
pipelines and Trondheim became my new buddies[2].

Networks and theory can be dry like the deserts,
and while performing a "double" proposal[3],
the audacity of hope for a "knack"[4] alike Dilbert's
and a helping advisor were at my disposal.

[2] I will happily remember the time I spend in your wonderful country, Bjarne, Tor, and Vidar. Mange takk for arbeide med meg!

[3] Mangala, thanks for the nnnnnnyes! ;)

[4] For more info on Erik's favorite youtube video, visit www.youtube.com and search the keywords "knack dilbert".

Subsurface flow, reservoirs, and water injection[5],
Nederland stay and weddings[6] were quite demanding.
Hence, in solitude of mathematical reflection,
the body of *network* knowledge was slowly expanding.

Café au lait[7], Belgian chocolates, and Lutefisk[8],
are essential ingredients for a balanced PhD.
The job market search was not without risk,
life lessons and support from Erik were key.

Now as we reach the final straight,
with Erik referring to the world's smartest man[9],
who never wrote anything and hence was his fate
that nobody knew all the things he can.

A *potential function* for a *network process*,
with a *gradient system's* differential equation,
makes *decentralized control* a final success,
and applies to *reservoirs* with good persuasion.

[5]Thank you, Jan Dirk, for everything you taught me about reservoir engineering, the support, and the fruitful discussions we had.

[6]Dear Amma and Seena uncle, dear Ajji and Raghu, and everyone from my Indian family: Thank you for the wonderful wedding in Bangalore, the support and love. You make me feel like I have always been part of your family.

[7]Sometimes, Erik and I would get a café au lait before an afternoon meeting, but we always felt guilty for having it in the afternoon.

[8]A traditional Norwegian Christmas dinner made from fish treated with lye. see http://en.wikipedia.org/wiki/Lutefisk

[9]According to Erik and Erik's father, the smartest man in the world lived in Chicago, but nobody knows it, since he never wrote up any of his genius into books or publications. This is how Erik used to motivate me to write up my ideas.

As a ”traveling salesman”[10] across the Atlantic,

optimizing my ”knapsack”[11] for frequent air carriage,

without friends[12] and family[13] I might have turned frantic,

and thank you, dear Mangala, for your love and our marriage[14].

Process Network Optimality:

Does it apply in all generality?

Is this the final finality?

It certainly misses some practicality,

but surely mirrors a bit of reality.

But certainly in its totality,

it might shift some minds and mentality.

Michael Wartmann

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[10]The traveling salesman problem is a problem in combinatorial optimization.

[11]The knapsack problem is a problem in combinatorial optimization. Thanks, Ignacio for teaching me about these optimization problems, being on my committee and many, many more things you supported me with.

[12]I would like to thank my very special friends I met in Pittsburgh (no particular order!) Tova, Anya, and Beni, Sarthak(wazaa!), Madhavi, Sebastian, Bistra and Steve, Sheetal and Achim, Lea and Juan, Willi, Trishna and Joey, Peter, Tanuka, Oxana, Tom, Julio and Fer, Tor, Ute and Nathan, Denis, Martina, Weanna, Fede and Fatos, Paul and Silvia, and Warren and Tank. Many thanks also to YRG, especially Juan. I am also grateful to the tennis people club, the McEnroes for some great tennis, and to Karen and Sean for teaching the best Hot Yoga in the world. Ich bin sehr froh darüber, gute Freunde in Deutschland zu haben. Liebe Kerstin, Marc, Heike, Flori and Senta, Daryll and Nils, Wolfi, Erik and Julia und Corinna, es freut mich, dass wir trotz meiner Abwesenheit immer in Kontakt geblieben sind. Veel dank aan mijn Nederlandse vrienden Alice, Rob and Charlie, Yus and Koen, en Martin, vooral ook dat jullie me een beetje Nederlands aangeleerd hebben!

[13]Vielen Dank liebe Eltern, Großeltern und Alina. Ohne Eure Unterstützung, Liebe und die Geduld von Euch allen während meiner Auslandsaufenthalte, wäre all dies nicht möglich gewesen.

[14]There is no way, I can ever thank you enough for your patience during the two years we were apart, the wonderful weddings, getting us our golden retriever puppy Fluffy and taking care of him while I was away and for all your love and support.

Nomenclature

Nomenclature for Theory Chapters 2 - 5

$\mathbf{A}$	fundamental node-to-branch cut set matrix
$\mathbf{A_R}$	fundamental node-to-branch cut set matrix for resistive flows
$\mathbf{A_T}$	fundamental node-to-branch cut set matrix for terminal flows
$\mathbf{C}$	matrix function of capacitive constitutive equations
E	storage function
f_{ij}	flow between nodes i and j
F_i	flow variable i
$F_{R,i}$	resistive flow variable i
$F_{T,i}$	terminal flow variable i
$F_{K,i}$	controlled flow i
$F_{M,i}$	measured flow i
$\mathbf{G}$	graph of process network
G	content
G^*	cocontent
J	flux
K_i	conductance of linear flow i
$\mathbf{M}$	fundamental mesh-to-branch loop matrix
n_f	number of flows
n_p	number of nodes
n_t	number of terminals
n_{faces}	number of faces
P	potential function
p_i	production rate at node i
R_i	resistance of linear flow i
S	entropy
t	time
u	control or input parameter

V	Lyapunov function or candidate function
w_i	potential at node i
W_i	potential difference of flow i
$W_{R,i}$	potential difference of resistive flow i
$w_{T,i}$	potential at terminal i
X	force
x_i	state variable at node i
y	measurement or output parameter
Z_i	inventory at node i
Z_i^c	setpoint for inventory control at node i
Λ	matrix function of resistive constitutive equations

Nomenclature for Liquid Flow in Porous Media Chapter 6

$\mathbf{A_x}$	connection matrix for flows in x-direction
$\mathbf{A_y}$	connection matrix for flows in y-direction
$c^{o,w,r}$	compressibility of oil, water, rock
$k^{o,w}(S^{o,w})$	relative permeability
$M_i^{o,w}$	mass of oil, water in grid block i
$\dot{M}_{x,y}^{o,w}$	mass flow of oil, water in x,y direction i
P_{pump}	power output of injector pump
p	pressure
p_Q	well pressure
q	recovery factor
$\dot{Q}_i^{o,w,PROD}$	production rate of oil, water at the production well i
$q^{o,w}$	well flow of oil, water
$S^{o,w}$	oil,water saturation of liquid phase
$\mathcal{S}^{o,w,r}$	specific entropy for the oil, water, rock phase

$\mathbf{T}$	transmissibility
T^q	time horizon to reach recovery factor
V^{liquid}	liquid volume
V^{total}	total volume
η^{int}	internal efficiency
η^{INJ}	injector efficiency
η^{PROD}	producer efficiency
$\mu^{o,w}$	viscosity of oil, water
$\vec{v}^{o,w}$	Darcy velocity of oil, water
$\rho^{o,w}$	density of oil, water
$\sigma^{o,w}$	dissipation through oil, water flow
σ_{valves}	power loss through control valves
ϕ	porosity
Ψ	reservoir potential function for pressure dynamics
Ψ^S	reservoir potential function for saturation dynamics

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Chapter 1

Introduction

"*Die Gedanken sind frei*."
German folk song

The control design and operation of complex interacting processes is a challenging task. Not only is it difficult to choose the proper variables to control and measure in a large system, it is also challenging to account for the dynamic interactions occurring across individual process units during operation [48]. The dynamics of the system often depends more on the topology and the arrangement of unit processes than the dynamics of the individual unit processes themselves [25]. Also, networks of processes are frequently impossible to model and optimize in a centralized fashion due to size and complexity.

It is common to decompose the control and optimization tasks of large process networks. Decentralized decision-making is frequently performed for a number of important reasons. It allows for flexibility towards changes in the system, redundancy, and robustness towards disturbances from outside [11]. However, the decomposition of a large process network into smaller subunits requires a good understanding of the objectives of local decision makers and how these influence overall per-

formance [18]. Although the decentralization of decision-making formally limits the effect of an individual control algorithm on the total system behavior, the dynamics of the process network resulting from interaction across units requires a type of information flow between the decentralized algorithms. In the ideal case, the general operational objective of a process network is incorporated in the structure of the decentralized control system such that control algorithms automatically adapt to changing conditions and uncontrolled parts of the process network self-optimize [47].

Hence, the question we ask is How can we connect the concept of local feedback control to the optimality conditions of an entire process network? Particularly, we are interested in cases in which certain types of control change the objective function of a network and thus how dynamics of the system are influenced when controllers or processes are added or taken away. Consider for example two processes as shown in Fig. 1.1A. Each process has a feedback controller which is an algorithm designed to meet some given stability and optimization targets. Our interest lies in investigating the effect of a physical connection on both processes forming a larger system in Fig. 1.1B. Under what conditions is the combination of the two processes stable? What is the resulting objective function of the combined system? What information has to be exchanged between the local control algorithms to guarantee robust, stable, and optimal operation?

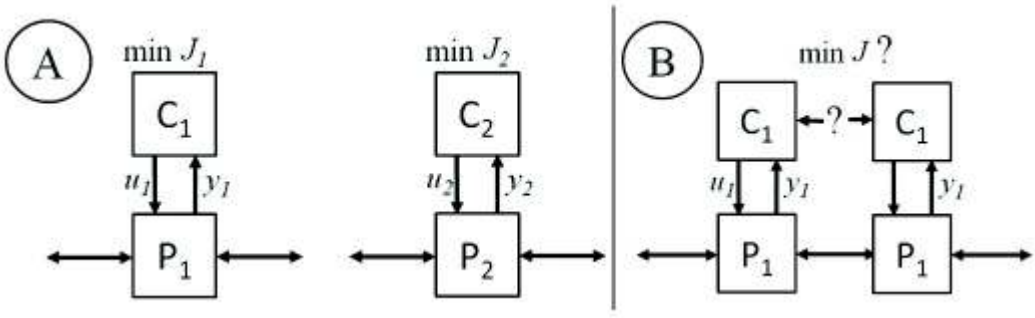

Figure 1.1: Two process systems P_1 and P_2 with individual control algorithms C_1 and C_2. The individual objective function of system 1 is J_1 and of system 2 is J_2. The physical connection of system 1 and 2 leads to a larger system where the objective function J and the information exchange between C_1 and C_2 are unknown.

In order to develop a good understanding of these concepts, we focus on distributed control of the inventories, i.e. quantifiable amounts such as mass and energy among others, at the nodes of a process network. In this way, we attempt to develop a flat rather than a hierarchical architecture for decentralized control and optimization. The approach we take is motivated by thermodynamic properties of the process network involving ideas from irreversible thermodynamics.

1.1 Processes and Irreversible Thermodynamics

Non-equilibrium thermodynamics naturally describes flow of energy, mass, or heat in processes, where at least one force gradient is upheld. These systems can only reach local equilibrium, since some of the potential gradients do not vanish due to external forces. The foundations of non-equilibrium thermodynamics were laid out by Maxwell [32], who introduced the minimum heat theorem stating that currents in electrical circuits take a path of minimum resistance, i.e., an electrical circuit self-minimizes the heat output.

The first comprehensive work however was published by Onsager [36, 37]. The motivation arose through the desire for consistent application of the second law, if the system is out of equilibrium. The second law of thermodynamics is here given as the positivity of local entropy production which is minimized when the system is in steady state:

$$\sigma_S = \sum_i J_i X_i \geq 0 \tag{1.1}$$

Entropy production is given by the product sum of the so called conjugate fluxes J_i and forces X_i in the system. In linear irreversible thermodynamics (LIT), each flux is a linear combination of all forces

$$J_i = \sum_j L_{ij} X_j \tag{1.2}$$

with the reciprocal relations being proven by Onsager [36, 37].

In order to apply concepts of non-equilibrium thermodynamics, extensive variables Z_i and the corresponding sets of conjugate fluxes $J_i = \frac{dZ_i}{dt}$ and forces $X_i = \frac{\partial S}{\partial Z_i}$ have to be identified. Prigogine [15] and Meixner [34] developed a systematic theory for non-equilibrium processes and determined the rate of entropy production for a number of relevant physical problems among them dissipative structures and transport processes in biology. Linking electrical systems to thermodynamics, Desoer and Vidyasagar [10] developed systematic network modeling methods for electrical circuits and analyzed stability properties of those based on passivity theory. Using a rigorous network modeling approach, Desoer and Kuh [9] and Oster, Desoer, Perelson, and Katchalsky [38, 39] developed a framework that combines the principles of electrical circuit theory with the framework of irreversible thermodynamics. Electrical circuits are of the best understood non-equilibrium systems studied and were the first type of physical system for which a variational principle based on dissipativity was discovered. Brayton and Moser derived a variational principle based on a mixed potential function for nonlinear electrical circuits [5, 6]. The Brayton-Moser equations describe an energy-based form of the dynamic equations for a wide class of nonlinear reciprocal systems using the gradient system:

$$\dot{Q}(x)\dot{x} = \nabla P(x) \tag{1.3}$$

where $Q(x)$ is a metric obtained from reversible elements and $P(x)$ is a mixed potential obtained from the irreversible constitutive equations. For the mixed potential, we have

$$P(X,J) = R(J) - G(X) + \Phi(J,X) \tag{1.4}$$

where $R(J)$ represents a function related to the content and co-content of the system. In a mechanical system, the content is related to the Rayleigh dissipation function. The potential function derived through the Brayton-Moser equations is one out of a large number of possible representations of a function linking dissipation, i.e., entropy production to a variational principle. In Chapter 3, we show

that a process network can be written as a gradient system on a similar form as the Brayton-Moser formulation in (1.3).

Generally, near equilibrium linear systems are well understood and the second law based on the dissipation function is well established. However, systems that are far from equilibrium are much harder to describe with variational principles, because in regions far from equilibrium, dynamics on other (smaller) time scales play an important role and constrain the system. In many cases, effects on smaller time scales can lead to bifurcation, if the system is driven out of the equilibrium state and hence to multiple pathways during transient motion. Several authors among them notably Jaynes [23] have stated that the inclusion of microscopic dynamics in the regarded macroscopic system leads to a behavior that selects the pathway most likely leading to minimum entropy production in the final state for non-equilibrium and to maximum entropy for equilibrium systems. This observation is supported by the work here provided that entropy production is defined to be equal to the cocontent described in Chapter 3.

1.2 Process Networks and Topology

A consistent modeling framework for arbitrarily complex process networks requires a consistent way of modeling the topological properties of the system. Oster and Desoer [38] pointed out that the topological foundations of network theory are identical to those of vector calculus which allows analysis of spatially discretized systems and leads to several advantages in the mathematical treatment. Firstly, a conceptual separation of reversible and irreversible elements is possible where the subsystems of the process network are either irreversible or reversible processes, each of which either dissipates energy or stores energy reversibly. Subsystems that contain both reversible and irreversible elements formally require that they can be decomposed into elementary purely capacitive or resistive elements. Secondly, a discretized system can directly be related to common numerical algorithms and compared to stability results that are based on systems of differential algebraic equations (DAE).

The most important advantage, however, is the compact and simple treatment of topological relations following from the conservation and continuity properties. The network treatment allows the application of matrix algebra instead of vector calculus which represent the same properties in the limit of infinitesimally small subunits [43]. Especially a result called Tellegen's theorem, acting as a topological invariant, allows a very compact derivation of many other results [42].

Tellegen's theorem itself constitutes a redundant equation on top of the continuity and conservation properties of physical networks and hence does not contribute directly towards determining the state or evolution of a process network. However, its compactness and the orthogonality property it describes between potential gradients and flows make it useful in different applications. In [25], Tellegen's theorem was derived for general process networks in order to be able to perform a global check of local decentralized controllers and hence demonstrate overall input-output stability. In this work, Tellegen's theorem assists in the proof of optimality conditions for process networks through a variational result, see Chapter 3.

Not only does Tellegen's theorem allow the very compact proof of important results, it also shows potential in serving as redundant constraint in the field of global optimization [53]. In recent years, global nonlinear optimization has made advances in the context of developing algorithms for different classes of problems. Some of these algorithms involve the use of redundant modeling constraints in order to improve the tightness of the convex relaxation generated by the optimization solver [29, 45]. Often, basic mass or energy balances can be violated for the relaxed problem, such that the addition of Tellegen's theorem to the model equations has the potential of enforcing the violated balances and thus assisting the optimization algorithm. The relevant theory and a global optimization example with Tellegen's theorem as a redundant constraint is given in Chapter 5.

1.3 Liquid Flow in Porous Media

The injection of a fluid to displace another fluid is a common process in petroleum production. In the most common application, fluids such as natural gas and oil are recovered through the injection of water to produce the hydrocarbons. Once the production rates decline due to decreasing pressure, the displacement process is called second recovery stage. During the displacement process, water is injected at fixed point sources, i.e., injection wells, in order to move a displacement front to a number of production wells. The position of these wells in the petroleum reservoir is typically determined heuristically during earlier recovery stages. Generally, the overall objective is to optimize some metric of the recovery efficiency by adjusting the flow rates or pressures at the injectors and producers. Key challenges for the efficient production through water injection are largely uncertain heterogeneity of the geological structure in combination with the nonlinearities of the two-phase flow behavior of the reservoir. It is therefore of interest to develop methods which are insensitive with respect to these uncertainties.

Recent studies have shown the potential of optimization strategies based on modeling and control technology for recovery techniques through water injection processes [22, 7, 58]. Closed-loop reservoir management, in which new information about the reservoir is repeatedly integrated into large scale models and optimal control type problems are used to enhance oil recovery. In most cases, an optimized strategy shows significant improvement, but is hard to implement from an operational point of view due to the frequent dynamic changes in the control settings. Simple thermodynamic principles as a basis for an efficient, reactive strategy using information from subsurface measurements and geology would be desirable as an intermediate solution between the conventional reactive strategy and an advanced closed-loop management solution based on detailed modeling. Linking displacement processes to a thermodynamic principle requires the use of non-equilibrium thermodynamics due to the transient nature and permanent pressure gradients across the physical domain of the reservoir.

Irreversible thermodynamics has been applied to liquid flow problems for groundwater and oil production, however, the focus has been on modeling rather than optimization and control. Karney and Seneviratne [27] illustrate the use of energy and entropy concepts for adaptive time step control in numerical simulation of liquid flow in porous media.

On the meso-scale, surface tensions between the fluids and the fluids and rock and sand formations play a significant role. Marle [31] and Pavone [41] developed methods that allow the consistent derivation of constitutive equations such as a generalized Darcy's law based on irreversible thermodynamics. They derived a macroscopic entropy balance equation based on effects on the meso-scopic level such as surface tensions, chemical reaction, and transport across phases and suggest how phenomenological equations have to be chosen for consistency across different time and length scales. However, these models most often are severely limited in the context of large scale numerical simulations or field optimization due to their complexity.

Our focus will be on giving insights into the application of irreversible thermodynamics for optimization of water injection for petroleum reservoirs and illustrating, under what conditions these principles hold. We will show how variational principles for process networks relate to optimality concepts for reservoir injection strategies in Chapter 6.

Chapter 2

Process Networks and Topology

”In nature we never see anything isolated,
but everything in connection with something else
which is before it, beside it, under it, and over it.”
Johann Wolfgang von Goethe

2.1 Process Networks

2.1.1 Interconnected Systems and (Redundant) Constraints

We consider dynamical systems which can be written as collections of interconnected sub-systems so that

$$\dot{x}_i = F(x_i) + \sum_{j=0}^{n} G(u_i, x_i, x_j), \quad i = 0, \ldots, n \tag{2.1}$$

$$w_i = H(x_i) \tag{2.2}$$

x_i is the state of subsystem i and $x_i(0)$ is the initial condition. The function F describes the unforced motion of the system, the function G describes how the system is connected with other sub-systems, and the output function H relates the state of the system to the evaluation functions w_i. We think of w_i as potentials or intensive variables for a process. These variables can be used to evaluate the performance of the process. The functions u_i represent the control parameters. The functions F, G, H are all differentiable at least once. The state of the entire network is given by the vector $\mathbf{x} = (\mathbf{x}_0^T, \mathbf{x}_1^T, ..., \mathbf{x}_n^T)^T$. Subscript zero refers to the reference (exo-)system.

Often we are not interested in the dynamics of the exo-system, or more likely, it is too complex to model. The network is then modeled as a reduced system without the exo-system. The interactions with the exo-system are then established through the boundary conditions as shown in Fig. 2.1. Examples of systems that can be modeled this way include chemical plants, supply chains, pipeline networks, flow through porous media, electrical circuits, metabolic reaction networks in biological systems, and many other systems of academic and practical interest.

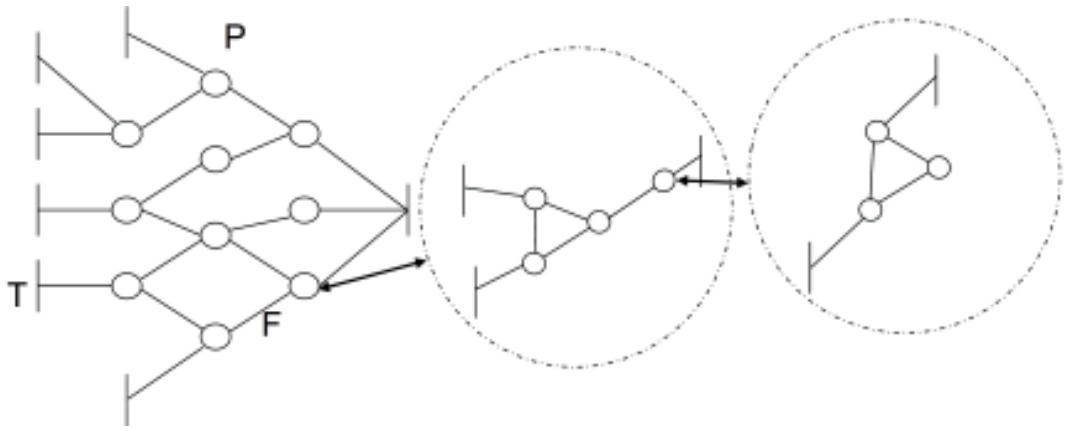

Figure 2.1: Graphical network representation: Topological structure of a network consisting of nodes P, terminals T, and flows F. Nodes contain subgraphs and give rise to a hierarchical multi-scale structure.

We now define a class of functions Z called the inventory of a sub-system or a group of systems. The inventory is a non-negative, additive function of the state of the corresponding sub-system(s). By additivity we mean that if Z_1 is the inventory of sub-system 1 and Z_2 is the inventory of sub-system

2, then $Z_1 + Z_2$ is the total inventory of the two subsystems. Hence for any i, j

$$Z\begin{pmatrix} x_i \\ x_j \end{pmatrix} = Z(x_i) + Z(x_j)$$

By non-negativity we mean that the inventory cannot be less than zero. Examples of physical inventories include mass, energy, and charge. More generally, an inventory is any property which is related to an amount. This can include financial and other assets included on a balance sheet used for accounting and reporting purposes.

By referring to (2.1) and using continuity we derive the conservation law

$$\frac{dZ_i}{dt} = p_i(x_i) + \sum_{j=1, j\neq i}^{n} f_{ij}(x_i, x_j, u) \tag{2.3}$$

The *drift*

$$p_i(x_i) = \frac{\partial Z(x_i)}{\partial x_i} F(x_i) \tag{2.4}$$

measures the rate of production of the inventories Z_i and the function

$$f_{ij}(x_i, x_j, u) = \frac{\partial Z(x_i)}{\partial x_i} G(u, x_i, x_j)$$

measures the supply of Z between sub-systems j and i. We have the symmetry condition

$$f_{ij}(u) = -f_{ji}(u)$$

The term

$$\phi(u, z, d) = \sum_{j=1, j\neq i}^{n} f_{ij}(u)$$

therefore measures the net rate of supply to sub-system i from all other sub-systems. It is called the

action on sub-system i. We make the assumption that the flows f_{ij} and the production p_i can be expressed as functions of the evaluation variables w_i, the difference of the evaluation variables W_{ij} for two different locations and control parameters u so that

$$f_{ij} = \hat{f}_{ij}(x, W_{ij}, w_i, u) \tag{2.5}$$

and

$$p_i = \hat{p}_i(x, w_i, u) \tag{2.6}$$

The differential equation (2.1) can be viewed as a constraint for the behavior of the much more complex dynamical system (2.1) and (2.2). For example, a simple overall mass balance for a large system is not needed to compute the dynamics, since the system itself ensures that the constraint is satisfied. Examples of very useful behavioral constraints include those derived for conservation principles, namely

- Mass balance
- Component balance
- Energy balance
- Balances for micro- and macroeconomics

Behavioral constraints can be very useful for the analysis and control of systems. Balance controls are of paramount importance in all kinds of systems, since the availability of amounts strongly constrains the degrees of freedom provided to a process or organization. Not only the availability but also the ability of moving the resources is relevant.

In this work, we are particularly interested in a special class of redundant constraints, namely those that can be derived by combining conservation laws with continuity principles. They hold for a special class of evaluation functions which can be thought of as intensive variables. One example for

such a constraint is the entropy of a system which in classical thermodynamics according to Gibbs is given by

$$S = \frac{1}{T}U + \left(\frac{p}{T}\right)V + \left(\frac{\mu}{T}\right)N \tag{2.7}$$

The entropy can be written as a product of a vector of intensive variables and extensive variables. Very rarely, if ever, is (2.7) used to compute the dynamics of a system. However, it is one of the most important equations in mathematical physics, since it provides some very firm constraints on how we expect systems to behave. In this sense, the entropy balance

$$\frac{\partial S}{\partial t} = -\frac{\partial}{\partial x}J_S + \sigma_S \tag{2.8}$$

where S is the entropy density per unit volume, J_S is the entropy flux and σ_S the entropy production per unit of volume, provides a (redundant) constraint. The entropy balance, however, is at a much higher level of abstraction than, e.g., the mass and energy balances.

The use of redundant constraints in process control and optimization has a long history. It provides the basis for important concepts like mass and energy balance control in dynamic systems and many steady state offline and real-time optimization systems.

2.1.2 Algorithms

We define the vectors of the latent (microscopic) state variables $\mathbf{x}$, the potentials $\mathbf{w}$, the flows $\mathbf{f}$, the potential differences $\mathbf{W}$, the inventories $\mathbf{Z}$, and the production rates $\mathbf{p}$. Consider the following relations

$$(\mathbf{x}, \mathbf{W}, \mathbf{w}) \mapsto \mathbf{f} \tag{2.9}$$

$$(\mathbf{x}, \mathbf{w}) \mapsto \mathbf{Z} \tag{2.10}$$

$$(\mathbf{x}, \mathbf{w}) \mapsto \mathbf{p} \tag{2.11}$$

Given variables $\mathbf{w}$ and potentially hidden or latent variables $\mathbf{x}$, we can calculate other variables $\mathbf{f}$, $\mathbf{Z}$, and $\mathbf{p}$. Such a calculation is called an algorithm. More abstractly, we define an algorithm as a relation

$$(x, y) \mapsto u \tag{2.12}$$

where x is called the state variable, y is called the output and u is called the input. We can for example use the linear algorithm

$$\begin{aligned} \mathbf{u} &= \mathbf{K}\mathbf{x} && (2.13)\\ \frac{d\mathbf{x}}{dt} &= \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u}\ ,\ \mathbf{x}(0) && (2.14)\\ \mathbf{y} &= \mathbf{C}\mathbf{x} && (2.15) \end{aligned}$$

which can be motivated by the linear optimal control problem

$$\min_{u} \int_0^{\infty} (\mathbf{y}^T\mathbf{y} + \mathbf{u}^T\mathbf{R}\mathbf{u}) ds \tag{2.16}$$

subject to (2.13), (2.14), and (2.15). The gain $\mathbf{K}$ is then given by solving the Riccati equations. In this work, we are interested in a general class of nonlinear algorithms which is said to be positive. There is no restriction on linearity since any function or operator which maps (x, y) to u can be used.

Definition 1. *The algorithm is said to be positive, if for any pairs* (u_1, u_2), (y_1, y_2) *we have*

$$(u_1 - u_2)(y_1 - y_2) \geq 0$$

In the linear case reported above, we have positivity, if

$$\mathbf{u}^T\mathbf{y} = \mathbf{x}^T\mathbf{C}^T\mathbf{K}\mathbf{x} \geq 0 \tag{2.17}$$

and hence, we require $\mathbf{C}^T\mathbf{K}$ to be positive semi-definite. In the more general case that we calculate u using a dynamic nonlinear operator, we require that $y \mapsto u$ is passive, i.e.

$$\int_0^\infty (u_1 - u_2)(y_1 - y_2) \geq -K > -\infty \tag{2.18}$$

Consider now an interconnected system of processes described by the equation

$$\frac{dZ_i}{dt} = p_i(x_i) + \sum_{j=1, j\neq i}^{n} f_{ij}(x_i, x_j, u)$$

We assume that we have a positive algorithm which evaluates potentials w so that we have

$$(w_1 - w_2)(Z_1 - Z_2) \geq 0 \tag{2.19}$$

In the simplest case, we can use linear algorithms:

$$cw_i = Z_i \tag{2.20}$$

$$f_{ij} = L_{ij}(Z_i - Z_j) \tag{2.21}$$

$$p_i = k_i w_i \tag{2.22}$$

The network is now called a process system [24].

2.2 Topological Properties

The isomorphism between discrete and continuous mathematical representations allows the use of graph theory to analyze dynamical systems through the separation of the dynamics into a kinematic (or topological) part and a dynamical one. This enables us to use topological results to derive results which are not trivial if we only use the dynamical description provided by (2.1).

2.2.1 Review of Graph Theory

A graph **G** is the finite set $\upsilon(\mathbf{G}) = (\upsilon_1, ...l, \upsilon_{n_p})$, whose elements are called **nodes**, together with the set $\varepsilon(\mathbf{G}) \subset \upsilon \times \upsilon$, whose elements are called **branches**. A branch is therefore an ordered pair of distinct nodes.

- If, for all $(\upsilon_i, \upsilon_j) \in \varepsilon(\mathbf{G})$, the branch $(\upsilon_j, \upsilon_i) \in \varepsilon(\mathbf{G})$ then the graph is said to be **undirected**. Otherwise, it is called a **directed graph**.
- A branch (υ_i, υ_j) is said to be **incoming with respect to** υ_j and **outgoing with respect to** υ_i and can be represented as an arrow with node υ_i as its tail and node υ_j as its head.

The incidence matrix gives a compact description of the topology of the network.

Definition 2. *The $n_t \times n_f$ matrix $\mathbf{N_a}$ is called node-to-branch incidence matrix for the matrix elements n_{ij} being*

$$n_{ij} = \begin{cases} 1, & \textit{if flow } j \textit{ is outgoing with respect to } i \\ -1, & \textit{if flow } j \textit{ is incoming with respect to } i \\ 0, & \textit{if flow } j \textit{ is not incident with node } i \end{cases}$$

One node of the network is set as reference or datum node P_0 to represent the exo-system. The $(n_t - 1) \times n_f$ matrix $\mathbf{N}$, where the row that contains the elements n_{0j} of the reference node P_0 is eliminated, is called reduced incidence matrix.

The connections between nodes through branches is uniquely defined by the incident matrix $\mathbf{N_a}$. $\mathbf{N_a}$ consists of n_p rows where only n_p-1 rows are linearly independent. It has n_b columns where each columns represents a branch and every non-zero element defines a connection to a node. One of the n_p rows represents the branches connecting the exo-system to the network nodes and can be seen as a linear combination of the first n_p-1 rows. Deleting the row of the datum node, the resulting matrix **N** contains n_p-1 independent rows.

Definition 3. *The $n_m \times n_f$ matrix $\mathbf{E_a}$ is called branch-to-mesh incidence matrix for the matrix elements e_{ij} being*

$$e_{ij} = \begin{cases} 1, & \textit{if flow } j \textit{ bounds mesh i in the + direction} \\ -1, & \textit{if flow } j \textit{ bounds mesh i in the - direction} \\ 0, & \textit{if flow } j \textit{ is not incident with mesh } i \end{cases}$$

A reference or outer mesh E_0 is part of the mesh structure and represents the exo-system. The $(n_m - 1) \times n_f$ matrix $\mathbf{E}$, where the row that contains the elements e_{0j} of the outer mesh E_0 is eliminated, is called reduced mesh incidence matrix.

The connection matrices $\mathbf{N}$ and $\mathbf{E}$ describe the kinematic or topological part of a dynamic process network model. Dual mathematical structures are available for the description of these properties and the concept of duality can be most conveniently illustrated through the dual pair of mesh and nodal incidence matrix. The important advantage of the discrete space model arises through the use of ordinary differential equations where contributions to the system behavior follow from the topology and dynamics which are conveniently separated. We introduce several important definitions for the structural characteristics of the regarded class of process networks.

Definition 4. *Process Networks:*

- *The network is connected if there exists at least one connection between any two nodes and terminal in the graph.*
- *A sub-graph $\mathbf{G}_i \in \mathbf{G}$ is a graph which has branches, nodes and terminals in one to one correspondence with the graph $\mathbf{G}$.*
- *A subgraph $\mathbf{L}$ of $\mathbf{G}$ is called a loop if it is connected and there are precisely two connections at each node.*

- *A subgraph* **T** *of* **G** *is called a tree if it is connected, contains all nodes in the graph, and contains no loop. A graph with n_p nodes has $n_p^{n_p-2}$ different trees.*
- *A tree is called a rooted tree if one node has been designated the root, in which case the branches have a natural orientation, towards or away from the root.*
- *The branches of* **G** *not in* **T** *are called Links.*
- *A cut node, or articulation point, is a node whose removal disconnects the remaining subgraph.*
- *A cut set, or node cut or separating set, is a set of nodes whose removal disconnects the remaining subgraph.*
- *A dual graph of a given planar graph* **G** *is a graph which has a node for each plane region of* **G**, *and a branch for each branch in* **G** *joining two neighboring regions, for a certain embedding of* **G**.
- *Any loop that surrounds a region without any branch reaching from the loop inside to such a region forms a face.*

The following theorem is called the fundamental theorem of graph theory.

Theorem 1. *Given a connected network with n_p elementary sub-systems, n_f connections and a tree* **T**.

- *There is a unique path between any two sub-systems.*
- *There are $n_t - 1$ connections in T and $n_l = n_f - n_p + 1$ links*
- *Every link of* **T** *and its unique connection defines a unique loop.*

The duality of extensive (inventories) and intensive (potentials) variables plays an important role in this work. The framework of graph theory enables us to express these duality concepts geometrically through the connection matrices. One of the prerequisites of the duality is the correct definition of the incident matrix, where the exo-system as the reference point is a center point of the resulting graph. For the concept of linear duality, the process network including the exo-system is required to fulfill the planarity condition, which is true only if the exo-system is connected to all subsystems of the process network.

Lemma 1. *Given a connected and planar network with n_p elementary sub-systems, n_f connections and n_t terminals, if the terminals and nodes of the network are connected to an additional node representing the exo-system, i.e., datum node, then the connections between the datum node and all terminals and nodes constitute fundamental flow connections and a rooted tree.*

Proof. Follows directly from Definition 4. □

Theorem 2. *If and only if a finite, connected, planar graph is drawn in the plane without any branch intersections, and n_p is the number of nodes, n_f is the number of branches and n_{faces} is the number of faces (regions bounded by branches, including the outer, infinitely-large region), then*

$$n_p - n_f + n_{faces} = 2 \tag{2.23}$$

Theorem 2 is the so called Euler characteristic. We use Euler's formula to prove the next theorem.

Theorem 3. *Given a connected and planar network* **G** *with n_p elementary sub-systems, n_f connections and n_t terminals, if the terminals and nodes of the network are connected to an additional node representing the exo-system, then the complete network consisting of the rooted tree about the reference node and the nodes of the network form a planar graph* $\mathbf{G}^*$.

Proof. The network **G** is planar and for its number of nodes, branches and faces we have $n_p - n_f + n_{faces} = 2$ from equation (2.23). The reference node adds one extra node, n_f branches and $n_p - 1$

faces to the graph which we call $\mathbf{G}^*$. We compute

$$n_p^* - n_f^* + n_{faces}^* = (n_p + 1) - (n_f + n_p) + (n_{faces} + n_p - 1) = 2 \tag{2.24}$$

□

A visual interpretation of the planarity of a graph is given by the image of a graph with no intersecting connections that can be drawn on a plane surface. The surface itself can be the surface of a sphere or other bodies as long as it is compact and the graph is drawn on only one side of the body. Fig. 2.2 illustrates how the addition of the exo-system adds one node to the graph but conserves planarity. Generally, a graph of a process network showing planarity in dimension n can be drawn on a hyperplane of dimension $n+1$ after addition of the exo-system, if the system is connected through a rooted tree. Special matrices are introduced with the property of the exo-system as the datum node.

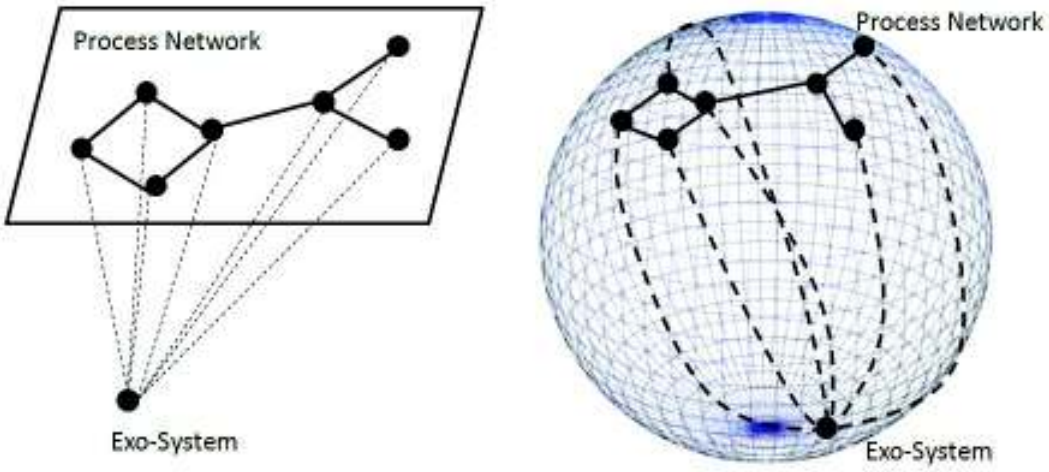

Figure 2.2: On the left: Planar process network. The exo-system is added as a node to provide a reference potential and connected to all subsystems. On the right: Although the process network cannot be drawn on a plane surface due to the reference node without intersecting branches, it can still be drawn on a sphere which shows planarity.

For these structures, the nodal and mesh connection matrices show orthogonality which will be shown in the following.

Definition 5. *The $n_t \times n_f$ matrix $\mathbf{A_a}$ is called node-to-branch fundamental cut set matrix for the matrix elements a_{ij} being*

$$a_{ij} = \begin{cases} 1, & \text{if flow } j \text{ belongs to cut set } i \\ & \text{and has the same reference direction} \\ -1, & \text{if flow } j \text{ belongs to cut set } i \\ & \text{and has the opposite reference direction} \\ 0, & \text{if flow } j \text{ does not belong to cut set } i \end{cases}$$

Corollary 1. *Given a rooted tree* $\mathbf{T}$ *which connects all sub-systems in the network to the reference node (the reference node in the center), we have a cut-set for every branch of the tree which results into a fundamental cut-set matrix* $\mathbf{A}$ *for the topology of the network.*

Proof. Proof follows immediately from Definitions 4 and 5, and Theorem 1. □

Definition 6. *The $n_t \times n_f$ matrix $\mathbf{M_a}$ is called branch-to-mesh fundamental loop matrix for the matrix elements M_{ij} being*

$$m_{ij} = \begin{cases} 1, & \text{if flow } j \text{ is in loop } i \\ & \text{and their reference direction agree} \\ -1, & \text{if flow } j \text{ is in loop } i \\ & \text{and their reference direction do not agree} \\ 0, & \text{if flow } j \text{ is not in loop } i \end{cases}$$

Corollary 2. *Given a rooted tree* $\mathbf{T}$ *which connects all sub-systems in the network to the reference node (the reference node in the center), we have a unique set of fundamental loops which are defined through the chosen tree* $\mathbf{T}$ *and its links between the tree branches. This results into a fundamental loop matrix* $\mathbf{M}$ *for the topology of the complete network.*

Proof. Proof follows immediately from Definitions 4, 5, and Theorem 1. □

2.2.2 Conservation Laws

The definition of the fundamental cut set **A** and loop matrix **M** allows the convenient formulation of inventory conservation since the conservation laws (2.3) can now be written

$$\mathbf{AF} = \mathbf{0} \tag{2.25}$$

for the node-to-branch incident matrix **A** where

$$\mathbf{F^T} = [\frac{dZ_1}{dt}, \frac{dZ_2}{dt}, ..., \frac{dZ_{n_p}}{dt}, f_{12}, f_{13} ... f_{n_{p-1},n_p}, p_1, ..., p_{n_p}]$$

we also have

$$\mathbf{F} = \mathbf{M}^T \mathbf{f} \tag{2.26}$$

for the mesh-to-branch incident matrix **M**. The flow vector **f** represents the so called fundamental flows which define a rooted tree. Each of the components of the vector **f**, i.e., each fundamental flow connects the exo-system in the center of the rooted tree to one of the nodes in the network. Equations (2.25) and (2.26) correspond to Kirchhoff's current law (KCL) of electrical circuit theory. The direction of the flows are defined according to the directionality established in the graph so that the flow is positive if it follows the direction of the graph and negative otherwise. Note that (2.25) is not sufficient to describe the complete behavior of system (2.1) and (2.3), it only provides a constraint on which behaviors can be observed.

2.2.3 Continuity of Potential Fields

For each node, we now define the potential vector $\mathbf{w} = [w_1..w_{n_p}]$ and $\mathbf{W}$ so that

$$\mathbf{W} = \mathbf{A}^T \mathbf{w} \tag{2.27}$$

for the node-to-branch incident matrix $\mathbf{A}$ and

$$\mathbf{MW} = \mathbf{0} \tag{2.28}$$

for the mesh-to-branch incident matrix $\mathbf{M}$, where $\mathbf{W}$ are the potential differences across flow connections. Due to the assumption of smoothness of the potential in the domain, it follows that for a discretized potential field the sum of potential differences along any closed loop

$$\sum_{LOOP} \Delta w_i = 0 \tag{2.29}$$

Kirchhoff's voltage law is equivalent to the statement that a single-valued potential can be assigned to each point in the domain (in the same way that any conservative vector field can be represented as the gradient of a scalar potential).

2.2.4 Tellegen's theorem

Theorem 4. ***Tellegen's theorem [9]****: Consider two networks (a) and (b) with the same topology (identical incidence matrix) but not necessarily the same state. Denote the variables in network (a) with the subscript a and denote variables in the other network with subscript b, then*

$$\mathbf{W}_b^T \mathbf{F}_a = \mathbf{W}_a^T \mathbf{F}_b = 0 \tag{2.30}$$

Proof. Node analysis:

$$\mathbf{W}_b^T \mathbf{F}_a = (\mathbf{W_b})^T \mathbf{F_a} \tag{2.31}$$

using KVL (2.27)

$$= (\mathbf{A}^T \mathbf{w}_b)^T \mathbf{F}_a \tag{2.32}$$

$$= (\mathbf{w}_b^T \mathbf{A}) \mathbf{F}_a \tag{2.33}$$

$$= \mathbf{w}_b^T \mathbf{A} \mathbf{F}_a = \mathbf{0} \tag{2.34}$$

since $\mathbf{A}\mathbf{F}_a = \mathbf{0}$ using KCL (2.25). □

The same result can be obtained by mesh analysis.

Proof. Mesh analysis:

$$\mathbf{W}_b^T \mathbf{F}_a = \mathbf{W}_b^T (\mathbf{F}_a) \tag{2.35}$$

using KCL (2.26)

$$= \mathbf{W}_b^T \mathbf{M}^T \mathbf{f}_a \tag{2.36}$$

$$= (\mathbf{M}\mathbf{W}_b)^T \mathbf{f}_a \tag{2.37}$$

$$= \mathbf{M}\mathbf{W}_b \mathbf{f}_a = \mathbf{0} \tag{2.38}$$

since $\mathbf{M}\mathbf{W}_b = \mathbf{0}$ using KVL (2.28). □

Lemma 2. *If the reference system, i.e., the datum node is disregarded, Tellegen theorem results in*

$$\mathbf{w}_b^T \frac{d\mathbf{Z}_a}{dt} = -\mathbf{W_R}_b^T \mathbf{F_R}_a - \mathbf{w_T}_b^T \mathbf{F_T}_a - \mathbf{w}_b^T \mathbf{p}_a \tag{2.39}$$

Proof. Details are shown in App. B, (2.39) corresponds to (B.22) and also follows directly from (2.30) □

Tellegen's theorem holds if the two Kirchhoff laws apply to the regarded model and states that the potential variables and the flow variables span orthogonal spaces. It holds for any two networks with the same topology even if they consist of different network elements. The constitutive equations may be nonlinear or linear, discrete or continuous, passive or active, and the network may have single or multiple steady states. The principle holds true even if we regard flows from a particular state t_1 and potentials from a particular state at time t_2 and vice versa. A version of Tellegen's theorem in summation form is given as

$$\sum_{i=1}^{n_p} \frac{dZ_i(t_1)}{dt} w_i(t_2) = -\sum_{i=1, i\neq j}^{n_f} f_{ij}(t_1)\Delta w_{ij}(t_2) + \sum_{i=1}^{n_t} f_{Ti}(t_1) w_{Ti}(t_2) + \sum_{i=1}^{n_p} p_i(t_1) w_i(t_2) \tag{2.40}$$

for two different states at times t_1 and t_2. If we consider a network ($a = b$) or a single state $t_1 = t_2$, then we can drop the superscript and we get the common form

$$\sum_{i=1}^{n_p} \frac{dZ_i}{dt} w_i = -\sum_{i=1}^{n_f} f_{ij}\Delta w_{ij} + \sum_{i=1}^{n_f} f_{Ti} w_{Ti} + \sum_{i=1}^{n_p} p_i w_i \tag{2.41}$$

which represents a power balance. This can also be seen in (B.22) of App. B. The term of the left hand side is an accumulation term $\sum_{i=1}^{n_p} \frac{dZ_i}{dt} w_i$ for the storage of potential energy in the nodes. On the right hand side, there are three terms for in- and outflux of power: Resistive terms for the energy dissipation induced by the flow process $\sum_{i=1}^{n_f} f_{ij}\Delta w_{ij}$, power input/output through in- and outflux of inventory at the terminals $\sum_{i=1}^{n_T} f_{Ti} w_{Ti}$, and production sinks and sources $\sum_{i=1}^{n_p} p_i(t_1) w_i(t_2)$. Tellegen's Theorem holds for cases in which transformations of the variables are allowed as long as they are transformed using network (Kirchhoff) operators [42]. The explicit derivation of Tellegen's theorem in summation form is given in App. B.

Definition 7. *Operators (Γ_Z,Γ_f,$\Gamma_{\Delta w}$,Γ_w) are called network operators if* (2.25) *and* (2.27) *hold for the transformed variables $\bar{Z} = \Gamma_Z Z, \bar{f}_{ij} = \Gamma_f f_{ij}, \Delta\bar{w}_{ij} = \Gamma_{\Delta w}\Delta w_{ij}, \bar{w}_{ij} = \Gamma_w w_{ij}$.*

Examples of acceptable network operators include time-averaging with finite, moving window,

discounting with exponential, linear filters, Fourier transforms, multiplication with constant matrices and vectors and linear forecasts based on past information [42]. The operators do not have to be linear, but linear ones are most often used in practical applications of Tellegen's Theorem.

The following theorem shows Tellegen's theorem in a more general form. It addresses the concept of duality and shows that once the topology of a network is fixed, we have graph invariants that allow us to transform mathematical formulations of a network using the concept of geometric duality.

Theorem 5. *[9] Call* $\mathbf{M}$ *the fundamental loop matrix and* $\mathbf{A}$ *the fundamental cut-set matrix of the same oriented graph, and let both matrices pertain to the same tree* $\mathbf{T}$*, then*

$$\mathbf{M}\mathbf{A}^T = \mathbf{0} \tag{2.42}$$

Proof. We have

$$\mathbf{W} = \mathbf{A}^T\mathbf{w}$$

and

$$\mathbf{M}\mathbf{W} = \mathbf{0}$$

combining both equations

$$\mathbf{M}\mathbf{A}^T\mathbf{w} = \mathbf{0}$$

This is only true for arbitrary $\mathbf{w}$, if $\mathbf{M}\mathbf{A}^T = \mathbf{0}$. □

The fundamental cut set matrix $\mathbf{A}$ can be partitioned so that

$$\mathbf{A} = \left[\begin{array}{cc} \mathbf{I}^{\mathbf{n_p}\times\mathbf{n_p}} & \mathbf{A_R} \end{array} \right]$$

where the nodes are represented through the identity matrix $\mathbf{I} \in \Re^{n_P \times n_P}$ and $\mathbf{A_R}$ represents the interconnection structure of resistive flows between the nodes. Analogously, the fundamental loop matrix

$\mathbf{M}$ can be decomposed into

$$\mathbf{M} = \begin{bmatrix} \mathbf{M_R} & \mathbf{I^{n_l \times n_l}} \end{bmatrix}$$

where $\mathbf{M_R}$ represents the position of the resistive flows in the network in particular loops being the identity matrix $\mathbf{I} \in \Re^{l \times l}$. The matrix $\mathbf{M_R}$ identifies the tree branches (either nodes or terminals) which are connected to the links (resistive branches).

Theorem 6. *For the decomposition of the fundamental cut set matrix* $\mathbf{A}$ *and the fundamental loop matrix* $\mathbf{M}$*, the internal structure of the matrices is as follows*

$$\mathbf{M} = \begin{bmatrix} -\mathbf{F}^T & \mathbf{I^{l \times l}} \end{bmatrix} \textit{ and } \mathbf{A} = \begin{bmatrix} \mathbf{I^{n_P \times n_P}} & \mathbf{F} \end{bmatrix}$$

Proof. We note that the fundamental cut set matrix are of the form

$$\mathbf{A} = \begin{bmatrix} \mathbf{I^{n_P \times n_P}} & \mathbf{A_R} \end{bmatrix} \text{ and } \mathbf{M} = \begin{bmatrix} \mathbf{M_R} & \mathbf{I^{l \times l}} \end{bmatrix}$$

Using Theorem 5

$$\mathbf{A}\mathbf{M}^T = \begin{bmatrix} \mathbf{I^{n_P \times n_P}} & \mathbf{A_R} \end{bmatrix} \begin{bmatrix} \mathbf{M_R}^T \\ \mathbf{I^{l \times l}} \end{bmatrix}$$

$$\mathbf{A}\mathbf{M}^T = \mathbf{I^{n_P \times n_P}}\mathbf{M_R}^T + \mathbf{A_R}\mathbf{I^{l \times l}} = \mathbf{0}$$

$$\mathbf{M_R}^T = -\mathbf{A_R}$$

If we call submatrix $\mathbf{A_R} = \mathbf{F}$, the result follows. □

2.2.5 Constitutive Relations

Constitutive equations are special cases of algorithms relating efforts and flows (resistive), flows and displacements (capacitive), and efforts and fluxes (inductive). The constitutive equations describe en-

ergy dissipating, irreversible processes (resistive) or energy storing, reversible processes (capacitive, inductive). They define the type of energetic transaction inside the network or between the system and the exo-system. We can consider them as algorithms as defined earlier and require positivity. The three main types can be described as

- Capacitive constitutive equation: storage of potential energy, $w = \hat{w}(Z)$
- Inductive constitutive equation: storage of kinetic energy, $p = \hat{p}(w)$
- Resistive constitutive equation: dissipation of energy, $f = \hat{f}(W)$

Fig. 2.3 shows the set of equations necessary to completely describe the network system and the connections between the variables. In many cases, typical models consist of a variety of capacitive,

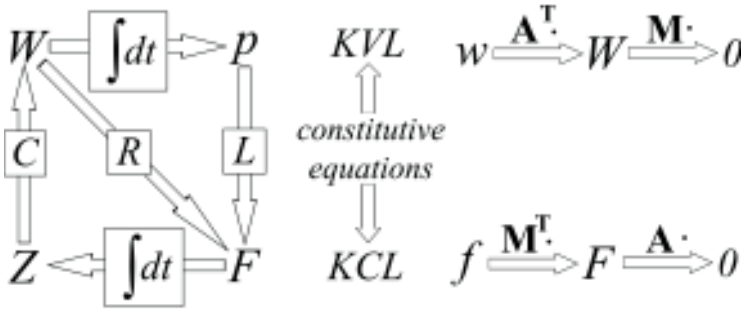

Figure 2.3: Graphical description of the state variables and their connections through constitutive equations. The variable p represents the impulse following from integrating the potential differences.

inductive, and dissipative constitutive equations which are often nonlinear and coupled. Typically, many different physical effects occur in networks and only some of them can be modeled consistently from first principles and in great detail, while other effects are captured through empirical model extensions and nonlinear approximations.

Different physical systems show similar characteristics in constitutive equations. In this work, we focus on systems with capacitive and resistive characteristics. Process systems are generally dissipative and kinetic energy storage (inductive model components) can often be neglected.

Example 1. *Electrical circuit: In an electrical circuit, the resistive constitutive equation is given by Ohm's law*

$$\Delta V_e = RI \tag{2.43}$$

relating the voltage difference ΔV_e across a linear resistor to the current through the resistor I. The resistor and Ohm's law form a dissipative connection element. The dissipation is given by the product of the effort and flow variable so that

$$\sigma = \Delta V_e I = RI^2 = \frac{1}{R}\Delta V_e^2 \tag{2.44}$$

The capacitive element in electrical circuit theory appears as

$$Q_e = CV_e \tag{2.45}$$

which models a linear capacitor. The capacitance relates the extensive variable charge Q_e to the intensive variable voltage V_e and presents a storage type constitutive equation. For electrical networks, the charges at the capacitors $Q_{e,i}$ correspond to the extensive variables or inventories Z_i, the voltages at the capacitors $V_{e,i}$ to the potentials w_i, and the electrical currents I_{ij} to the flows f_{ij}. Tellegen's theorem for an arbitrary electrical circuit follows as

$$\sum_{i=1}^{n_C} \frac{dQ_{e,i}}{dt} V_{e,i} = -\sum_{i=1}^{n_f} I_{ij}\Delta V_{e,ij} + \sum_{i=1}^{n_f} P_{e,i} \tag{2.46}$$

where $P_{e,i}$ are the power sources at the terminals.

In the following, we will focus describing constitutive equations as a linear or nonlinear relationship between the flow variables F_i and the potentials w_i or potential differences W_i of the form $\mathbf{F} = \Lambda(\mathbf{W})$ or $\Lambda(\mathbf{W},\mathbf{F}) = 0$ in its implicit form. The general flow vector representation $\mathbf{F}^T = [\frac{d\mathbf{Z}}{dt}^T, \mathbf{F_T}^T, \mathbf{F_S}^T, \mathbf{F_R}^T]$ contains sub-vectors representing the storage $\frac{d\mathbf{Z}}{dt}$, the source or sink terms

$\mathbf{F_S}^T = [\mathbf{F_T}^T, \mathbf{p}^T]$ in form of terminals and production, and the resistive flow connections $\mathbf{F_R}$. We represent the constitutive equations in the form

$$\mathbf{F} = \Lambda(\mathbf{W} - \mathbf{W_S}) + \mathbf{F_S} \tag{2.47}$$

including elements for storage, source/sink, and resistive flow in the explicit form given as

$$\begin{aligned}
\frac{\mathbf{dZ}}{\mathbf{dt}} &= \mathbf{C}\frac{d\mathbf{w}}{dt} && (2.48)\\
\mathbf{F_S} &= [\mathbf{F_T}, \mathbf{p}]^T && (2.49)\\
\mathbf{W_S} &= \mathbf{w_T} && (2.50)\\
\mathbf{F_R} &= \mathbf{G}\mathbf{W_R} && (2.51)
\end{aligned}$$

The matrix form of the set of constitutive equations can be captured using a diagonal matrix according to [9]

$$\begin{bmatrix} \frac{\mathbf{dZ}}{\mathbf{dt}} \\ (\mathbf{1}-\mathbf{d_T})\mathbf{F_T} \\ \mathbf{p} \\ \mathbf{F_R} \end{bmatrix} = \begin{bmatrix} \mathbf{C}\frac{d}{dt} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{d_T} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{G} \end{bmatrix} \left(\begin{bmatrix} \mathbf{w} \\ \mathbf{w_T} \\ \mathbf{0} \\ \mathbf{W_R} \end{bmatrix} - \begin{bmatrix} \mathbf{0} \\ \mathbf{w_S} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} \right) + \begin{bmatrix} \mathbf{0} \\ (\mathbf{1}-\mathbf{d_T})\mathbf{F_T} \\ \mathbf{p(t)} \\ \mathbf{0} \end{bmatrix} \tag{2.52}$$

The matrix representation leads to a compact and generalized description of the constitutive equations. The vector of decision variables $\mathbf{d_T}$ allows the choice for the terminal conditions to be either fixed in the flows $\mathbf{F_T}$ or the potentials $\mathbf{w_T}$ or mixed boundary conditions. The terminal potential is given for $d_{Ti} = 1$ and the terminal flow is fixed for $d_{Ti} = 0$.

2.3 Flow Network Example

The network consists of two connected pipelines where each pipeline flows through a cylindrical storage tank with volume V_j, as shown in Fig. 2.4. The system is connected to its surroundings at the tanks and at the outlet terminal which are open to the atmosphere. Each pipeline's cross section is cylindrical with area A_j. The pipeline flow is given as a lumped parameter representation introducing pressure potentials p_j at the nodes. It is assumed that the fluid shows Newtonian behavior as well as being incompressible ($\rho = \text{const.}$). The relation between volumetric flow $\dot{V}_i$ and pressure drop Δp_i can be modeled using different types of constitutive equations from the linear case of Hagen-Poiseuille's law

$$\dot{V}_i = \frac{\pi r_i^4}{8\eta L_i}\Delta p_i \tag{2.53}$$

to more complex functions as for example polynomials, i.e., quadratic and cubic relationships which represent valves and special geometries of the pipes

$$\dot{V}_i = \frac{\pi r_i^4}{8\eta L_i}(a_n \Delta p_i^n + a_{n-1}\Delta p_i^{n-1} + \ldots + a_0) \tag{2.54}$$

where r_i is the radius of the pipeline's cross-section and L_i is the length of pipeline i. The pressure at the bottom of the tank is given as

$$p_j = \rho g h_j + p_{atm} \tag{2.55}$$

by hydrostatics. The fluid volume V_j in the tank is connected to the level h_j through $V_j = A_j h_j$ where A_j is the cross-section of the tank. The system obeys Kirchhoff's voltage law in the pressures, i.e.,

smoothness of the pressure along the pipeline-system. We have

$$\begin{aligned} \Delta p_1^{IN} &= p_{T1} - p_1 && (2.56)\\ \Delta p_2^{IN} &= p_{T1} - p_2 && (2.57)\\ \Delta p_1^{OUT} &= p_1 - p_{T2} && (2.58)\\ \Delta p_1^{OUT} &= p_2 - p_{T2} && (2.59) \end{aligned}$$

We complete the model with the conservation laws for mass or, for constant density, the conservation of volume:

$$\begin{aligned} dV_1/dt &= \dot{V}_1^{IN} - \dot{V}_1^{OUT} && (2.60)\\ dV_2/dt &= \dot{V}_2^{IN} - \dot{V}_2^{OUT} && (2.61)\\ \dot{V}_{T1} &= \dot{V}_2^{IN} + \dot{V}_2^{IN} && (2.62)\\ \dot{V}_{T2} &= \dot{V}_2^{OUT} + \dot{V}_2^{OUT} && (2.63) \end{aligned}$$

Initial conditions for the tank volumes $V_{0,i}$ have to be specified as well as boundary conditions at the terminals. The dynamic trajectory of (2.53) - (2.63) can be found by integrating the differential equations. Tellegen's theorem for the example results in a power balance for

$$\mathbf{F}^T = [\frac{dV_1}{dt}, \frac{dV_1}{dt}, \dot{V}_{T1}, \dot{V}_{T2}, \dot{V}_1^{IN}, \dot{V}_1^{OUT}, \dot{V}_2^{IN}, \dot{V}_2^{OUT}]$$

and the potential vector as

$$\mathbf{W}^T = [p_1 - p_{atm}, p_2 - p_{atm}, p_{T1}, p_{T2}, \Delta p_1^{IN}, \Delta p_1^{OUT}, \Delta p_2^{IN}, \Delta p_2^{OUT}]$$

as

$$p_1 \frac{dV_1}{dt} + p_2 \frac{dV_2}{dt} = - \Delta p_1^{IN} \dot{V}_1^{IN} - \Delta p_1^{OUT} \dot{V}_1^{OUT} + p_{T1} \dot{V}_{T1} \quad (2.64)$$

$$- \Delta p_2^{IN} \dot{V}_2^{IN} - \Delta p_2^{OUT} \dot{V}_2^{OUT} + p_{T2} \dot{V}_{T2} \quad (2.65)$$

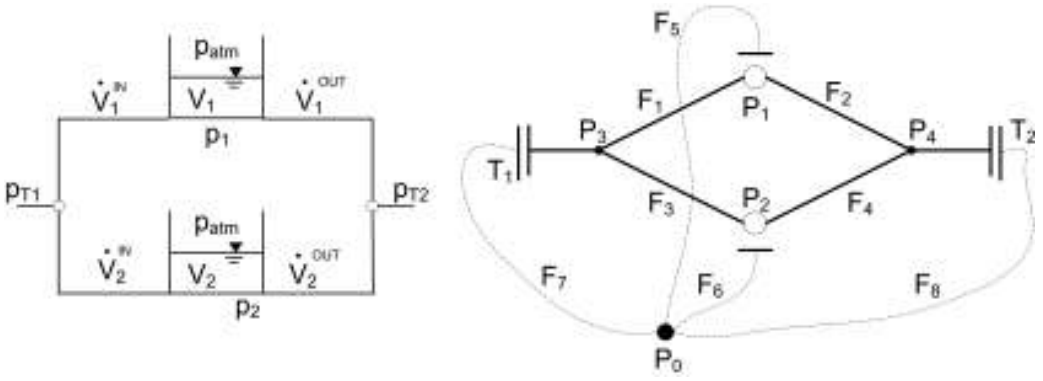

Figure 2.4: Graphical network representations: On the left, the problem specific representation shows connected pipelines in parallel where each pipeline flows through a storage tank. On the right, a generalized representation of the pipeline network is given consisting of nodes P_1 - P_4 (tanks P_1 - P_2 and junctions P_3 - P_4), pipelines F_1 - F_4 and inflow and outflow terminals T_1 and T_2. A reference node P_0 is introduced to represent the environment.

The flow network has the property that the connections between the reference node and the network nodes define a tree which allows the convenient construction of the topology matrices, as shown in Figure 2.4 and 2.5. A key property of these networks is that a fundamental tree with the reference node in the center can always be constructed by definition and dissipative elements only appear in the links. The fundamental cut set matrix can be constructed from the fundamental cut sets in Fig. 2.5.

$$\mathbf{A_a} = \begin{array}{c} \begin{matrix} F_1 & F_2 & F_3 & F_4 & F_5 & F_6 & F_7 & F_8 \end{matrix} \\ \begin{bmatrix} 1 & 0 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & -1 & -1 \\ -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array} \begin{matrix} P_1 \\ P_2 \\ P_3 \\ P_4 \\ P_0 \end{matrix}$$

The fundamental loop matrix is

$$\mathbf{M_a} = \begin{array}{c} \begin{matrix} F_1 & F_2 & F_3 & F_4 & F_5 & F_6 & F_7 & F_8 \end{matrix} \\ \begin{bmatrix} 1 & 0 & -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 \end{bmatrix} \end{array} \begin{matrix} P_1 \\ P_2 \\ P_3 \\ P_4 \\ P_0 \end{matrix}$$

The reduced fundamental matrices are obtained if we delete the row of the datum node for the fundamental cut set matrix and the row of the outer mesh for the fundamental loop matrix. The fundamental cut set matrix $\mathbf{A}$ consists of

$$\mathbf{A} = \begin{bmatrix} \mathbf{I^{4\times 4}} & \mathbf{A_R} \end{bmatrix}$$

where

$$\mathbf{A_R} = \begin{bmatrix} -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & -1 & -1 \end{bmatrix}$$

represents the resistive flow connections to nodes and terminals. The fundamental loop matrix de-

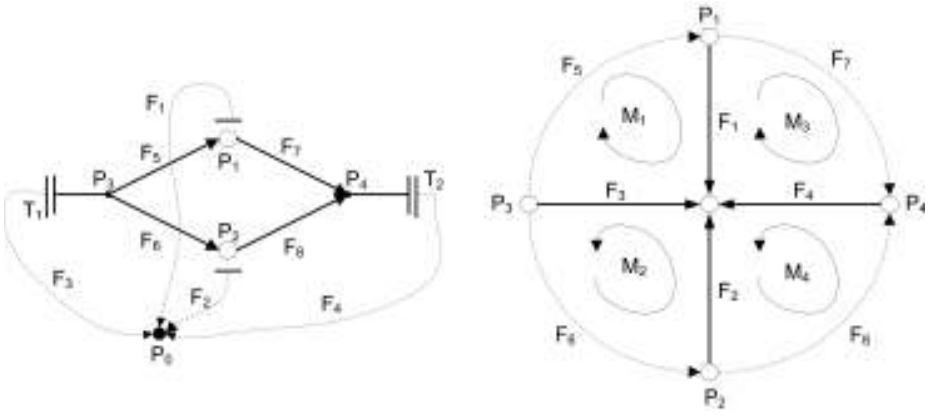

Figure 2.5: Constructing a planar graph representation and defining trees and links. The solid flow connections in the figure represent the fundamental tree where the dashed lines are the link connections. Connections between the tree branches through one link form fundamental loops. The graph is used to construct the fundamental cut set matrix **A** and the fundamental loop matrix **M**.

composes as follows:

$$\mathbf{M} = \begin{bmatrix} \mathbf{M_R} & \mathbf{I^{4\times 4}} \end{bmatrix}$$

where

$$\mathbf{M_R} = \begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & -1 & 0 \\ -1 & 0 & 0 & 1 \\ 0 & -1 & 0 & 1 \end{bmatrix}$$

represents the loops including the links (resistive branches).

The set of matrix constitutive equations in the form of $\mathbf{F} = \Lambda(\mathbf{W} - \mathbf{W_S}) + \mathbf{F_S}$ follows as

$$\begin{bmatrix} \frac{dV_1}{dt} \\ \frac{dV_1}{dt} \\ (1-d_{T1})\dot{V}_{T1} \\ (1-d_{T2})\dot{V}_{T2} \\ \dot{V}_1^{IN} \\ \dot{V}_1^{OUT} \\ \dot{V}_2^{IN} \\ \dot{V}_2^{OUT} \end{bmatrix} = \Lambda \left(\begin{bmatrix} p_1 \\ p_2 \\ p_{T1} \\ p_{T2} \\ \Delta p_1^{IN} \\ \Delta p_1^{OUT} \\ \Delta p_2^{IN} \\ \Delta p_2^{OUT} \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \\ p_{s1} \\ p_{s2} \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \right) + \begin{bmatrix} 0 \\ 0 \\ (1-d_{T1})\dot{V}_{s1} \\ (1-d_{T2})\dot{V}_{s2} \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{2.66}$$

where

$$\Lambda = \begin{bmatrix} \frac{A_1}{\rho g}\frac{d}{dt} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{A_2}{\rho g}\frac{d}{dt} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & d_{T1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & d_{T2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\pi r_{1,IN}^4}{8\eta L_1^{IN}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\pi r_{1,OUT}^4}{8\eta L_1^{OUT}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{\pi r_{2,IN}^4}{8\eta L_2^{IN}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\pi r_{2,OUT}^4}{8\eta L_2^{OUT}} \end{bmatrix}$$

2.4 Thermodynamic Processes

Let Σ be a convex sub-set of $\mathbb{R}^n_+$ and let $\mathbf{Z} = (Z_1, ..., Z_n)$ represent an arbitrary point. A vector $\mathbf{Z}$ can be regarded as the inventory of n different properties of the system. We distinguish between two types of inputs and outputs. The signals, y and u, represent measured outputs and control inputs.

We now define a class of $\mathbb{C}_1$ functions $\varepsilon(Z) : \Sigma \longmapsto \mathbb{R}_+$ called extensions. An extension is said to be conserved if its rate of production equals zero. It is dissipative if its production is less or equal to zero and it satisfies the Clausius−Planck inequality if its rate of production is greater or equal to zero [57]. Mass and energy are examples of extensions that satisfy all these properties. The entropy of classical thermodynamics satisfies the Clausius−Planck inequality. These extensions used in passivity theory are called storage or dissipation functions and they satisfy the dissipation inequality [8].

Definition 8. *A system with conservation laws* (2.3) *is called a process system if there exist extensions* $S(Z)$ *and* $E(Z)$ *so that*

1. *S(Z) is concave in Z.*
2. *S(Z) is positively homogeneous of degree one in Z.*
3. *E(Z) is conserved and* $T = \frac{\partial E}{\partial S} > 0$.

The function $S(Z)$ *is called the entropy, the function* $E(Z)$ *is called the energy and* T *is called the temperature.*

Formally, the optimality and stability conditions derived in this work are explained for a special class of systems incorporating only one inventory type Z, i.e., one set of conjugate variables. In the electrical analogue, we have the conjugate variables voltage and current, for pipeline flow, volumetric flow and pressure. We present a range of systems and physical effects that can be captured using the

Process	**Inventory** Z	**Potential** w	**Flux** F	**Resistive** $F = f_R(W)$	**Capacitive** $w = f_C(Z)$
Circuit	Charge Q_e[C]	Voltage U_e[V]	Current I[A]	$\Delta U_e = RI$	$Q_e = CU_e$
Liq. pipe-tank-flow	Volume V[m^3]	Pressure p[Pa]	Vol. flow $\dot{V}$[m^3/s]	$\dot{V} = \frac{\pi r^4}{8\eta L}\Delta p$	$p = \rho g\frac{V}{A} + p_0$
Heat conduction (isochoric)	Internal Energy U[J]	Temperature T[K]	Heat flow $\dot{Q}$[W]	$\dot{Q} = -kA\frac{\Delta T}{\Delta x}$	$dU = c_V dT$
Diffusion network	Amount N_i[mol]	Concentration ϕ_i[mol/m^3]	Diffusion flux J_i[mol/m^{2}s]	$J_i = -D\frac{\Delta\phi_i}{\Delta x}$	$N_i = \phi_i V$
Reaction network	Amount N_i[mol]	Affinity a[mol/m^3] $=-\sum_i \nu_i\mu_i$	Reaction rate r_i[mol/m^{2}s]	$r_i = f(a)$	$\mu_i = \mu_i^0 + RT\ln\frac{N_i}{N}$

Table 2.1: Constitutive equations for different types of processes.

process network modeling framework. For more examples of conjugate variables, see Table 2.1 which gives an overview over some typical process systems in relation to network theory.

If we integrate different types of inventories such as

$$\mathbf{Z_i}^T = (U_i, V_i, M_{i,1}, ..., M_{i,n_c}, A_i, Q_{i,e})$$

and their corresponding intensive variables

$$\mathbf{w_i}^T = \left(\frac{1}{T_i}, \frac{p_i}{T_i}, \frac{\mu_{i,1}}{T_i}, ..., \frac{\mu_{i,n_c}}{T_i}, \frac{\sigma_i}{T_i}, \frac{V_{i,e}}{T_i}\right)$$

for each node i then the conservation laws and uniqueness conditions can be extended into tensors and matrices. The conservation laws

$$\frac{dZ_i}{dt} = \sum_{j=1}^{b^{IN}} f_{ij}^{IN} - \sum_{j=1}^{b^{OUT}} f_{ij}^{OUT} + \sum_{j=1}^{p} p_i \quad i = 1, ..., n_V \tag{2.67}$$

at each node can be connected through the production terms p_i which transform different types of inventories into each other, i.e., several components react to products and release energy, or, in a supply chain case, different assets are assembled into a finalized product. The framework requires to regard the sink/source term p_i as a terminal to connect one type of inventory to a different inventory through a transformer. In terms of the conservation laws, we have

$$\begin{aligned}
\mathbf{A_1 F_1} &= \mathbf{0} \\
\mathbf{A_2 F_2} &= \mathbf{0} \\
&\vdots \\
\mathbf{A_{n_i} F_{n_i}} &= \mathbf{0}
\end{aligned} \tag{2.68}$$

Eq. (2.68) corresponds to Kirchhoff's current law in a generalized form so that the extensive variables $\mathbf{Z}$ can be a matrix of the dimension $\mathbb{R}^{n_p \times n_I}$, where n_p is the number of nodes and n_I the number of different inventories. In compact form, (2.68) can be written as

$$A_{ijk} F_{jk} = 0_{ik} \tag{2.69}$$

where A_{ijk} is an incident tensor and the node index i enumerates the number of nodes n_p, the branch index j the number of flows n_f, and the inventory index k the number of inventories n_I. Analogously, we have

$$M_{ijk} W_{jk} = w_{ik} \tag{2.70}$$

Tellegen's theorem follows directly as

$$A \otimes M = 0 \tag{2.71}$$

In case we have a system of different inventories Z_A, Z_B, ... , Z_{n_I} where transformation occurs at certain nodes, the network equations and Tellegen's theorem also applies for each individual species as in (2.68). The terminals have been defined as connections to the exo-system assuming one of the two conjugate terminal variables as constant or an explicit function of time. For the case of transformation of one inventory species into another, additional flow connections are defined that link the individual species networks at certain nodes, see Fig. 2.6 for a transformation species A and B to C. Here, the linked transformation terminals are connected through an additional node in

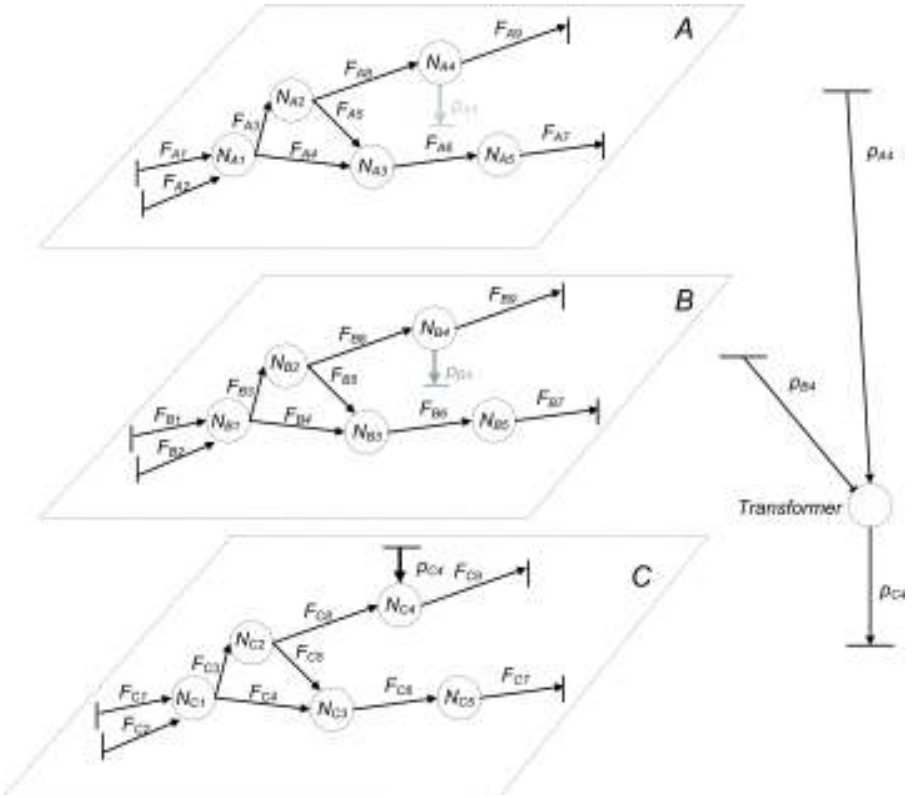

Figure 2.6: Transport and transformation in a three level network with three different species A, B, and C. The reactive nodes have transformation terminals and are connected to a reaction network.

which the transformation occurs. For the reversible parts of the transformation such as $A \rightarrow B$ the transformation occurs through the equations

$$\begin{bmatrix} p_A \\ w_A \end{bmatrix} = \begin{bmatrix} r & 0 \\ 0 & -1/r \end{bmatrix} \begin{bmatrix} p_B \\ w_B \end{bmatrix} \tag{2.72}$$

For the irreversible parts, as for example in chemical reactions, a concept of gradient induced flow can be introduced using the concept of chemical affinity of chemical resistors. The constitutive equation between reaction progress J_r and chemical affinity α

$$J_r = f_R(\alpha) \tag{2.73}$$

The reaction flows can be represented through the stoichiometric matrix ν for molar flows p_i resulting in the equivalent of Kirchhoff's current law.

$$\nu \mathbf{p_i} = \mathbf{0} \tag{2.74}$$

The definition of chemical affinity for a certain reaction is

$$\alpha = -\nu\mu \tag{2.75}$$

Each transformation is hence a combination of a dissipative flow and an ideal transformer. Tellegen's theorem for a number of different species follows as

$$\sum_{i=1}^{n_c} \mathbf{F_i}^T \mathbf{W_i} = 0 \tag{2.76}$$

In the extended form, we have

$$\sum_{i=1}^{n_c} \mathbf{F_{i,R}^T} \mathbf{W_{i,R}} + \sum_{i=1}^{n_c} \mathbf{F_{i,T}}^T \mathbf{w_{i,T}} + \sum_{i=1}^{n_c} \frac{d\mathbf{Z_i}}{dt}^T \mathbf{w_i} + \sum_{i=1}^{n_c} \mathbf{p_i}^T \mathbf{w_i} = 0 \tag{2.77}$$

and for cross connections between different species

$$\alpha^T \mathbf{J_r} + \sum_{i=1}^{n_c} \mathbf{p_i}^T \mathbf{w_i} = 0 \tag{2.78}$$

where the first term corresponds to the dissipation of every individual reaction. We can substitute (2.78) into (2.77)

$$\sum_{i=1}^{n_c} \mathbf{F_{i,R}}^T \mathbf{W_{i,R}} + \sum_{i=1}^{n_c} \mathbf{F_{i,T}}^T \mathbf{w_{i,T}} + \sum_{i=1}^{n_c} \frac{\mathbf{Z_i}}{dt}^T \mathbf{w_i} + \alpha^T \mathbf{A} \mathbf{J_r} = 0 \tag{2.79}$$

.

Example 2. *Continuous stirred tank reactor (CSTR): We consider a CSTR with exothermic reaction in liquid media in which a reversible reaction of the reactant A to the product B takes place:*

$$A \rightleftharpoons B$$

The stoichiometric coefficient is given as 1. We have balance equations for the following vector $\mathbf{Z}^T = [U, V, N_A, N_B]$ *of extensive quantities with the corresponding potentials* $\mathbf{w}^T = [T, p, c_A, c_B]$*. The balances for the extensive variable vector are given as:*

Balance of extensive variables:

$$\frac{d\mathbf{Z}}{dt} = \mathbf{Z}^{IN} - \mathbf{Z}^{OUT} + p_{\mathbf{Z}} \tag{2.80}$$

Energy-related constitutive equations:

$$U = \sum_{i=A,B,I} N_i [c_{v,i}(T - T_{ref}) + U_{ref}] \tag{2.81}$$

$$H^{IN,OUT} = \rho c_P (T^{IN,OUT} - T_{ref}) \tag{2.82}$$

$$U^{IN,OUT} = F^{IN,OUT} * H^{IN,OUT} \tag{2.83}$$

$$p_U = Q + rV(-\Delta H_r) \tag{2.84}$$

The energy related constitutive equations are characterized as a function of the temperature T as a measurable intensive variable. We describe the energy U as a function of the temperature and the volume where we have

$$dU = \left(\frac{\partial U}{\partial V}\right)_T dT + \left(\frac{\partial U}{\partial T}\right)_T dV$$

We assume the changes in energy as a function of the volume small compared to the temperature and also $c_V = \left(\frac{\partial U}{\partial V}\right)_T = const$. *We regard the enthalpy similarly as*

$$dH = \left(\frac{\partial H}{\partial p}\right)_p dT + \left(\frac{\partial U}{\partial T}\right)_T dp$$

and assume that the change in the pressure contribution to the energy is negligible. These approximations which are very common in chemical engineering models lead us to the capacitive constitutive equations (2.81) *and* (2.82). *Equation* (2.83) *is necessary as a definition in order to consistently formulate the process network framework. Volume related constitutive equations:*

$$F^{IN} = K_{IN}(p^{IN} - p) \tag{2.85}$$

$$F^{OUT} = K_{OUT}(p - p^{OUT}) \tag{2.86}$$

$$V = \frac{\rho g}{A}(p - p_0) \tag{2.87}$$

$$p_V = 0 \tag{2.88}$$

The volume related constitutive equations define the flow rates based on the pressure as potential variable. In (2.85) *and* (2.86) *we have resistive constitutive equations for the pressure driven flow. Equation* (2.87) *describes a relationship between the volume V and the pressure p based on hydro-*

statics. Component balance related constitutive equations:

$$N_A = c_A V \tag{2.89}$$

$$N_B = c_B V \tag{2.90}$$

$$F_A^{IN} = c_A^{IN} F^{IN} \tag{2.91}$$

$$F_B^{IN} = c_B^{IN} F^{IN} \tag{2.92}$$

$$F_A^{OUT} = c_A F^{OUT} \tag{2.93}$$

$$F_B^{OUT} = c_B F^{OUT} \tag{2.94}$$

$$p_A = -Vr \tag{2.95}$$

$$p_B = Vr \tag{2.96}$$

$$r = k_A c_A - k_B c_B \tag{2.97}$$

The definitions of the concentrations c_A and c_B in (2.89) *and* (2.90) *are classical examples of capacitive constitutive equations. These equations are bilinear due to the fact that the volume V is a dynamic variable. The equations* (2.91)*,* (2.92)*,* (2.93)*, and* (2.94) *define the relationship between component flow and total flow for the process network framework. Similarly, the reaction behavior requires the definitions for p_A and p_B and another resistive constitutive equation is given through* (2.97)*.*

Chapter 3

Optimality and Stability Conditions for Process Networks

”Nature is an endless combination and repetition of a very few laws.

She hums the old well-known air through innumerable variations.”

Ralph Waldo Emerson

3.1 Network Content and Cocontent

The content $G(i)$ and the cocontent $G^*(v)$ of a nonlinear resistor are defined as

$$G(i) = \int^i v(i)di \tag{3.1}$$

$$G^*(v) = \int^v i(v)dv \tag{3.2}$$

according to Millar [35]. The content and cocontent of a nonlinear resistor in its geometrical significance [42] can be shown in Fig. 3.1. The lower limits of content and cocontent need not be specified

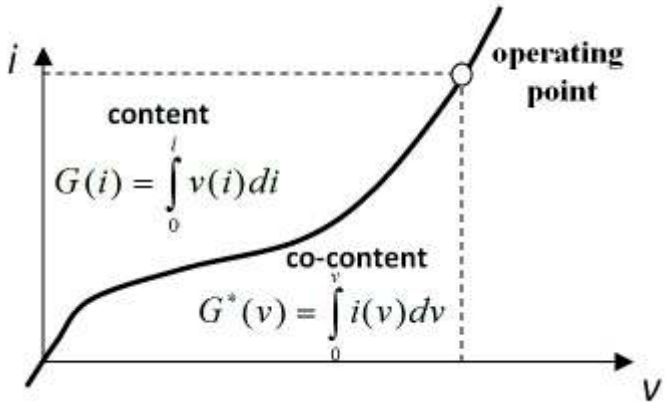

Figure 3.1: The content and cocontent are equal to the areas above and below the characteristic curve of the resistor.

until the functions are actually evaluated. Commonly, they are taken as the points $i = 0$ for the content or $v = 0$ for the cocontent. For the content and cocontent we assume local symmetry

$$\frac{\partial v_1}{\partial i_2} = \frac{\partial v_2}{\partial i_1} \tag{3.3}$$

The assumption of local symmetry is necessary and sufficient so that content and cocontent are only dependent on the end points and not the path of integration [42]. Under the assumption of local symmetry, it follows that the content $G(i)$ is a locally concave function of i and the cocontent $G^*(v)$ is a locally convex function of v. This notion can be extended towards general convexity if the positivity condition for the resistor holds

$$(v_1 - v_2)(i_1 - i_2) \geq 0 \tag{3.4}$$

Adding the content and cocontent gives the total dissipation σ

$$\sigma = G(i) + G^*(v) = iv \tag{3.5}$$

We define the content as in (3.1) of a node as the indefinite integral

$$G_{R,i} = \int^{F_{R,i}} W_{R,i} dF_{R,i} + \int^{p_i} w_i dp_i \tag{3.6}$$

The cocontent as in (3.2) is given as

$$G^*_{R,i} = \int^{W_{R,i}} F_{R,i} dW_{R,i} + \int^{w_i} p_i dw_i \tag{3.7}$$

The total dissipation of one node follows as

$$\sigma_i = G_{R,i} + G^*_{R,i} = W_{R,i} F_{R,i} + p_i w_i \tag{3.8}$$

and the total dissipation for the entire process network

$$\sigma = \sum_{i=1}^{n_f} (G_{R,i} + G^*_{R,i}) = \sum_{i=1}^{n_f} W_{R,i} F_{R,i} = \mathbf{W_R}^T \mathbf{F_R} + \mathbf{w}^T \mathbf{p} \tag{3.9}$$

For a network with a graph $\mathbf{G}$, we can define the network content

$$G = \sum_{i=1}^{b} \int^{F_i} W_i dF_i = \int^{\mathbf{F}} \mathbf{W}^T d\mathbf{F} \tag{3.10}$$

and the network cocontent

$$G^* = \sum_{i=1}^{b} \int^{W_i} F_i dW_i = \int^{\mathbf{W}} \mathbf{F}^T d\mathbf{W} \tag{3.11}$$

The network content G and cocontent G^* represent the sum of contents and cocontents for **all** types

of branches, i.e., reversible, irreversible, production and terminal flow connections of the network.

Lemma 3. *For the network content G and the cocontent* G^*

$$G^*(\mathbf{W}) = \min_{\mathbf{F}}(\mathbf{W}^T\mathbf{F} - G(\mathbf{F})) \tag{3.12}$$

Equation (3.12) is a form of Tellegen's theorem and it shows that G^* and G are dual variables where a change of variables between $\mathbf{W}$ and $\mathbf{F}$ corresponds to a Legendre transformation (see Fig. 3.1).

Lemma 4. *For the sum of network content* $G = \int^{\mathbf{F}} \mathbf{W}^T d\mathbf{F}$ *and network cocontent* $G^* = \int^{\mathbf{W}} \mathbf{F}^T d\mathbf{W}$*, the following relation holds:*

$$G + G^* = 0$$

Proof. The result follows immediately from Tellegen's theorem and Lemma 3. □

The concept of the content and cocontent can be generalized which can then further include non-symmetric algorithms relating flows and potentials [35]. The generalized cocontent for the process network system is defined as

$$G^*(t) = \int_0^T \mathbf{F}^T \frac{d\mathbf{W}}{dt} dt \tag{3.13}$$

which shows how the cocontent can be transformed into a line integral. In this form, the cocontent depends on the past history of the process network, but also assumes a state function if local symmetry of the algorithms is assumed [42]. The content can be generalized similarly.

Theorem 7. *The cocontent in form of a line integral*

$$G^* = \int_0^T \mathbf{F}^T \dot{\mathbf{W}} dt$$

is given as

$$G^* = \left[\mathbf{F}^T\mathbf{W}\right]_T - \int_0^T \mathbf{W}^T\dot{\mathbf{F}}dt$$

Proof. Through integration by parts, we obtain:

$$G^* = \left[\mathbf{F}^T\mathbf{W}\right]_T - \left[\mathbf{F}^T\mathbf{W}\right]_0 - \int_0^T \mathbf{W}^T\frac{d\mathbf{F}}{dt}dt$$

The result follows for a proper choice of initial conditions for which the initial cocontent is zero. □

3.2 First Order Conditions and Duality

It can be shown through Tellegen's theorem, that the content and cocontent assume an extremal point for a state in which the process network is stationary [38]. For the regarded process network, Tellegen's theorem is given as $\mathbf{W}^T\mathbf{F} = 0$. If we perturb the currents by $d\mathbf{F}$, Tellegen's theorem results in

$$\mathbf{W}^T(\mathbf{F} + d\mathbf{F}) = 0 \tag{3.14}$$

Subtracting Tellegen's theorem from (3.14) we have $\mathbf{W}^T d\mathbf{F} = 0$. Since, the terminal currents are constant, the perturbations vanish and it follows

$$dG_R^* = \mathbf{W_R}^T\delta\mathbf{F_R} = 0 \tag{3.15}$$

The perturbations are also perpendicular to the space of the potential differences and thus, at the steady state, the cocontent is stationary. Alternatively, a similar analysis can be carried out for constant potentials at the boundaries for the content.

Although (3.15) shows a powerful result, it is difficult to connect it to a particular description of a network. Therefore, we focus in the following on developing the first order conditions for an opti-

mization problem as a complete description of a process network. Based on Tellegen's theorem and the content and cocontent, we propose an optimization problem that allows us to find the steady state and dynamic trajectory of a dynamic process network. This optimization problem has to correspond exactly to a set of network equations of the process network **G** such as in

$$\mathbf{AF} = \mathbf{0} \tag{3.16}$$

$$\mathbf{W} = \mathbf{A}^T\mathbf{w} \tag{3.17}$$

$$\mathbf{F}-\mathbf{F_S} = \Lambda(\mathbf{W}-\mathbf{W_S}) \tag{3.18}$$

with the three main sets of constraints: Conservations laws (2.25), uniqueness conditions (2.28), and the constitutive equations (2.47) are defined in Chapter 2.

3.2.1 Optimization Duality: Node-based Analysis

In the following theorem, we introduce the connection between content, cocontent, and the Kirchhoff laws, and present how duality of the free variables plays a crucial role for the optimization problem solved when process networks converge to steady state.

Theorem 8. *For the optimization problem describing the variational principle of a process network*

$$\min_{\mathbf{w}} \quad G^* = \int_0^W \mathbf{F}^T d\mathbf{W} \tag{3.19}$$

$$s.t. \qquad \mathbf{W} = \mathbf{A}^T\mathbf{w} \tag{3.20}$$

$$\mathbf{F} = \Lambda(\mathbf{W}) \tag{3.21}$$

the Lagrange multipliers follow as the process network's flow variables **F**.

Proof. We first substitute the constitutive equations (3.21) into the objective function (3.19) to elim-

inate the flow variables $\mathbf{F}$. The Lagrange function of the resulting optimization problem is

$$\min L(\mathbf{W},\mathbf{w},\lambda) = \int_0^W \Lambda(\mathbf{W})^T d\mathbf{W} + \lambda^T(\mathbf{A}^T\mathbf{w} - \mathbf{W}) \tag{3.22}$$

The first order optimality conditions are given by

$$\begin{aligned} \frac{\partial L}{\partial \mathbf{W}} &= \Lambda(\mathbf{W}) - \lambda = \mathbf{0} && (3.23)\\ \frac{\partial L}{\partial \mathbf{w}} &= \mathbf{A}\lambda = \mathbf{0} && (3.24)\\ \frac{\partial L}{\partial \lambda} &= \mathbf{A}^T\mathbf{w} - \mathbf{W} = \mathbf{0} && (3.25) \end{aligned}$$

comparing (3.23) and the constitutive equations (3.21), it follows that $\lambda = \mathbf{F}$. Using $\lambda = \mathbf{F}$ in (3.23) and (3.24), the result follows. □

We note that if we have a complete set of network equations as in (3.16), (3.17), and (3.18), then the objective function given through the cocontent is formally redundant. Removing one set of Kirchhoff laws (either the current or the voltage law) allows to formulate an optimization problem where the omitted Kirchhoff law is recovered, see Fig. 3.2. The optimization problem with the Kirchhoff voltage law as constraints can be converted to an optimization problem with the Kirchhoff current law and vice versa.

Theorem 9. *The optimization problem describing the process network as a function of the potentials* $\mathbf{w}$ *as optimization variables*

$$\begin{aligned} \min_{\mathbf{w}} \quad & G^* = \textstyle\int_0^W \mathbf{F}^T d\mathbf{W} && (3.26)\\ s.t. \quad & \mathbf{W} = \mathbf{A}^T\mathbf{w} && (3.27)\\ & \mathbf{F} = \Lambda(\mathbf{W}) && (3.28) \end{aligned}$$

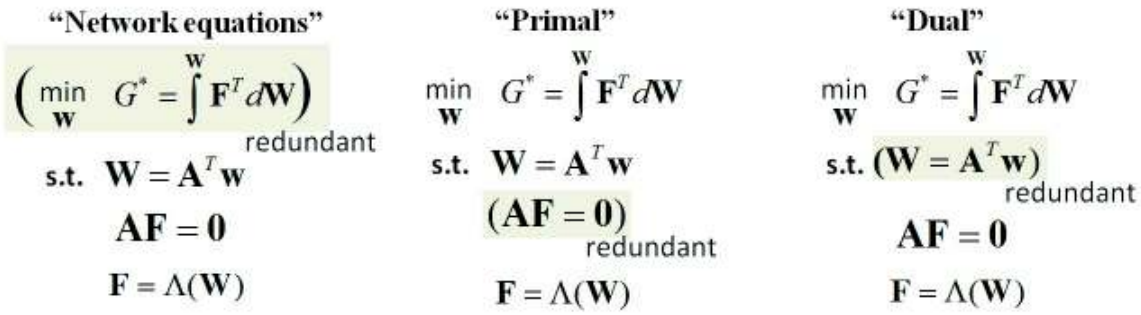

Figure 3.2: On the left, classical network equations where the cocontent is redundant and not necessary for describing the system. In the middle, the primal problem is given where Kirchhoff's current law is redundant. On the right, the dual problem describes the system where Kirchhoff's voltage law is redundant.

is equivalent to the optimization problem as a function of the flow variables $\mathbf{F}$

$$\min_{\mathbf{F}} \quad G^* = \int_0^W \mathbf{W}^T d\mathbf{F} \tag{3.29}$$

$$s.t. \qquad \mathbf{AF} = \mathbf{0} \tag{3.30}$$

$$\mathbf{F} = \Lambda(\mathbf{W}) \tag{3.31}$$

with the content G^* *as objective function, the conservation laws, and resistive constitutive equations as constraints.*

Proof. Starting with

$$\min_{\mathbf{W}} \quad G^* = \int_0^W \mathbf{F}^T d\mathbf{W} \tag{3.32}$$

$$s.t. \qquad \mathbf{W} = \mathbf{A}^T\mathbf{w} \tag{3.33}$$

$$\mathbf{F} = \Lambda(\mathbf{W}) \tag{3.34}$$

and moving the uniqueness condition into the objective function with the flows $\mathbf{F}$ as Lagrangean

multipliers

$$\min \quad L = \int_0^W \mathbf{F}^T d\mathbf{W} + \mathbf{F}^T(\mathbf{A}^\mathbf{T}\mathbf{w} - \mathbf{W}) \tag{3.35}$$

$$s.t. \qquad \mathbf{F} = \Lambda(\mathbf{W}) \tag{3.36}$$

we rearrange the objective function

$$\min \quad L = \int_0^W \mathbf{F}^T d\mathbf{W} - \mathbf{W}^T\mathbf{F} + \mathbf{w}^T\mathbf{A}\mathbf{F} \tag{3.37}$$

$$s.t. \qquad \mathbf{F} = \Lambda(\mathbf{W}) \tag{3.38}$$

using Tellegen's theorem (3.12), we substitute all terms containing $\mathbf{W}$ and carry out a variable transformation

$$\min \quad L = \int_0^F \mathbf{W}^T d\mathbf{F} - \mathbf{w}^T\mathbf{A}\mathbf{F} \tag{3.39}$$

$$s.t. \qquad \mathbf{F} = \Lambda(\mathbf{W}) \tag{3.40}$$

We can now treat $\mathbf{w}$ as a Lagrange multiplier and move the term $\mathbf{AF}$ back into the set of constraints.

$$\min \quad L = \int_0^F \mathbf{W}^T d\mathbf{F} \tag{3.41}$$

$$s.t. \qquad \mathbf{A}\mathbf{F} = \mathbf{0} \tag{3.42}$$

$$\mathbf{F} = \Lambda(\mathbf{W}) \tag{3.43}$$

□

The theorem shows the duality of flows $\mathbf{F}$ and potentials $\mathbf{w}$ and the duality between different formulations of the optimization problem. The concepts can be understood as the classical duality encountered in many optimization problems such as in linear or quadratic programming. The opti-

mality principle based on potentials w as free variables and the cocontent G^* can be understood as the primal problem while the flows F as free variables and the content G as the dual problem. It is easy to show that the dual of the dual results in the primal. The duality theorem states that if either the primal or the dual problem has a finite solution, then so does the other and their values are equal under the assumption that the constitutive equations are bijective and strictly monotonous, see Chapter 2, Section 2.1.2.

3.2.2 Optimization Duality: Mesh-based Analysis

The dual problem based on the fundamental loop matrix $\mathbf{M}$ can be proven analogously.

Theorem 10. *For the optimization problem describing the variational principle of a process network*

$$\max_{\mathbf{f}} \quad G = \int_0^F \mathbf{W}^T d\mathbf{F} \tag{3.44}$$

$$s.t. \qquad \mathbf{F} = \mathbf{M}^T \mathbf{f} \tag{3.45}$$

$$\mathbf{W} = \Omega(\mathbf{F}) \tag{3.46}$$

the Lagrange multipliers follow as the process network's potential differences $\mathbf{W}$.

Proof. Proof analogously to Theorem 8. □

Theorem 11. *The optimization problem describing the process network as a function of the fundamental flows* $\mathbf{f}$ *as optimization variables*

$$\max_{\mathbf{f}} \quad G = \int_0^F \mathbf{W}^T d\mathbf{F} \tag{3.47}$$

$$s.t. \qquad \mathbf{F} = \mathbf{M}^T \mathbf{f} \tag{3.48}$$

$$\mathbf{W} = \Omega(\mathbf{F}) \tag{3.49}$$

is equivalent to the optimization problem as a function of the potential differences $\mathbf{W}$

$$\max_{\mathbf{W}} \quad G = \int_0^F \mathbf{F}^T d\mathbf{W} \tag{3.50}$$

$$s.t. \qquad \mathbf{MW} = \mathbf{0} \tag{3.51}$$

$$\mathbf{W} = \Omega(\mathbf{F}) \tag{3.52}$$

Proof. Proof analogously to Theorem 9. □

3.2.3 Topological Duality

Theorem 12. *The optimization problem*

$$\min_{\mathbf{f}} \quad G = \int_0^F \mathbf{W}^T d\mathbf{F} \tag{3.53}$$

$$s.t. \qquad \mathbf{F} = \mathbf{M}^T \mathbf{f} \tag{3.54}$$

$$\mathbf{W} = \Omega(\mathbf{F}) \tag{3.55}$$

is equivalent to

$$\min_{\mathbf{F}} \quad G = \int_0^F \mathbf{W}^T d\mathbf{F} \tag{3.56}$$

$$s.t. \qquad \mathbf{AF} = \mathbf{0} \tag{3.57}$$

$$\mathbf{F} = \Lambda(\mathbf{W}) \tag{3.58}$$

Proof. Pre-multiplication of (3.54) and the inverse mapping $\Omega^{-1} = \Lambda$ assuming bijectivity of constitutive equations (see Chapter 2 Section 2.1.2) and the result follows. □

Theorem 13. *The optimization problem*

$$\min_{\mathbf{w}} \quad G^* = \int_0^W \mathbf{F}^T d\mathbf{W} \tag{3.59}$$

$$s.t. \qquad \mathbf{W} = \mathbf{A}^T \mathbf{w} \tag{3.60}$$

$$\mathbf{F} = \Lambda(\mathbf{W}) \tag{3.61}$$

is equivalent to

$$\min_{\mathbf{W}} \quad G^* = \int_0^W \mathbf{F}^T d\mathbf{W} \tag{3.62}$$

$$s.t. \qquad \mathbf{M}\mathbf{W} = \mathbf{0} \tag{3.63}$$

$$\mathbf{W} = \Omega(\mathbf{F}) \tag{3.64}$$

Proof. Proof analogously to Theorem 12. □

We encounter a second form of duality which addresses the topological properties of the process network as shown in Chapter 2. The previous results show that there is an intrinsic connection between the duality in the optimization sense and the topological duality. Fig. 3.3 shows the relationship between the two encountered types of duality in process networks. We can identify four different optimization problems that are equivalent and interconnected, i.e., duals of one another. Small examples for the different dual problems are given in Section 3.3.1 after the introduction of the second order conditions. Luenberger [30] describes several important versions of duality such as topological duality between graphs, duality found in linear programming, and the duality of observability and controllability. The findings in this work show that these types of duality are related for process networks.

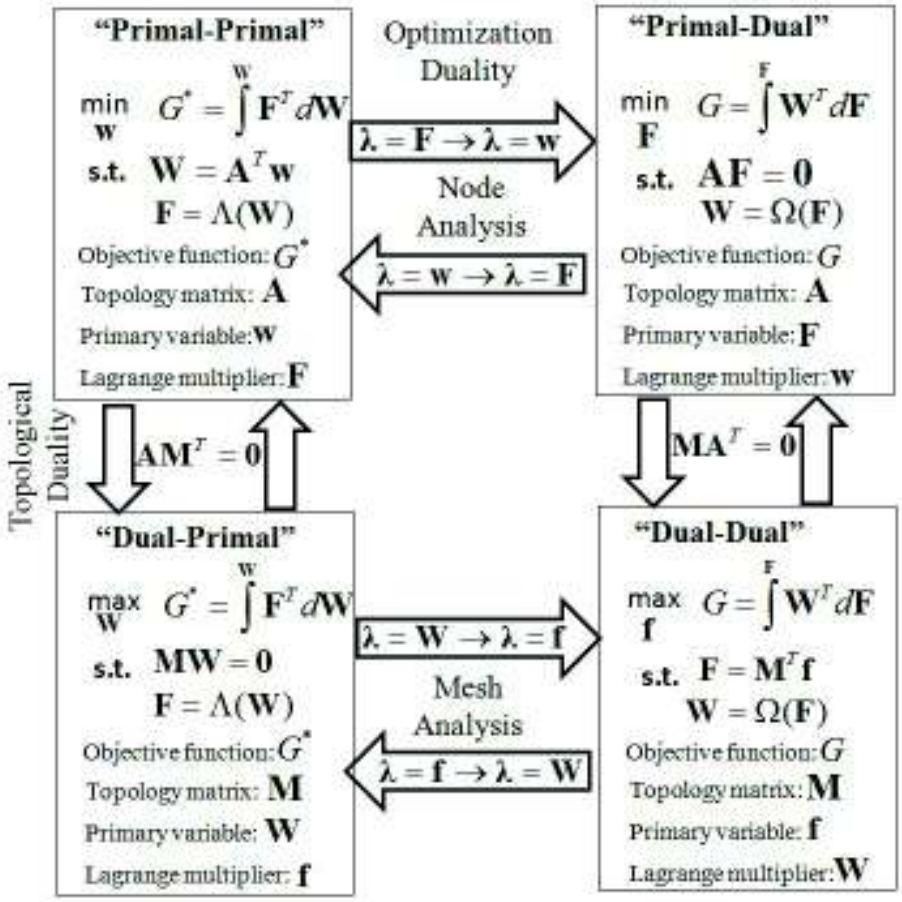

Figure 3.3: Duality principles of process networks: Duality in optimization between flow variables and potential variables (optimization duality) as Lagrangean multipliers of one another and structural duality between flow and potential variables (topology duality) due to the connection between mesh and node representations.

3.2.4 Variational Principle with fixed Terminal Conditions

We now propose the main theorem which allows the connection of the state of a process network to the optimization problem simultaneously optimized, i.e., we can find the natural optimization problem that a network solves, when converging on a certain trajectory. The following theorem shows the minimum entropy production principle for a general process network connected to the exo-system. The boundary conditions are incorporated through (2.47).

Theorem 14. *Consider a network* **G** *as defined in Chapter 2. The solution for the network with conservation laws and the uniqueness conditions*

$$\mathbf{AF} = \mathbf{0} \tag{3.65}$$

$$\mathbf{W} = \mathbf{A^T w} \tag{3.66}$$

$$\mathbf{F} - \mathbf{F_S} = \Lambda(\mathbf{W} - \mathbf{W_S}) \tag{3.67}$$

can be found by solving the following optimization problem

$$\min_{\mathbf{w}} \quad G^* = \int_0^W \mathbf{F}^T d\mathbf{W} \tag{3.68}$$

$$s.t. \quad \mathbf{W} = \mathbf{A^T w} \tag{3.69}$$

$$\mathbf{F_R} = \Lambda(\mathbf{W_R}) \tag{3.70}$$

$$\mathbf{F_T} = const \text{ and/or } \mathbf{w_T} = const \tag{3.71}$$

or its equivalent dual optimization problem where (3.66) is replaced by (3.65). Conversely, the solution of the optimization problem (3.68) - (3.71) *can be found by solving the differential equations* (3.65) - (3.67) *which corresponds to the method of steepest descent.*

Proof. Starting with (3.68) - (3.71), we substitute the boundary conditions (3.71) into the constitutive equations (3.70) and the constitutive equation into the objective function (3.68). We then form the

Lagrange function using the flows $\mathbf{F}$ as Lagrange multipliers

$$L(\mathbf{W},\mathbf{w},\mathbf{F}) = \int_0^W (\Lambda(\mathbf{W}-\mathbf{W_T})d\mathbf{W}+\mathbf{W}^T\mathbf{F_T} \tag{3.72}$$

$$+ \mathbf{F}^T(\mathbf{A^T w}-\mathbf{W}) \tag{3.73}$$

The first order optimality conditions are given by

$$\frac{\partial L}{\partial \mathbf{W}} = \Lambda(\mathbf{W}-\mathbf{W_T})+\mathbf{F_T}-\mathbf{F}=\mathbf{0} \tag{3.74}$$

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{AF}=\mathbf{0} \tag{3.75}$$

$$\frac{\partial L}{\partial \mathbf{F}} = \mathbf{A^T w}-\mathbf{W}=\mathbf{0} \tag{3.76}$$

□

Comparing (3.16) - (3.18) to (3.74) - (3.76) shows the result. Several examples of process networks are given in Section 3.3.1 following the analysis of the second order conditions of the content and cocontent formulations and their effect on stability and optimality properties of process networks.

Similarly, the analysis can be performed using the content and the topology given through using mesh analysis.

Theorem 15. *Consider a network* $\mathbf{G}$ *as defined in Chapter 2. The solution for the network with conservation laws and the uniqueness conditions*

$$\mathbf{MW} = \mathbf{0} \tag{3.77}$$

$$\mathbf{F} = \mathbf{M}^T\mathbf{f} \tag{3.78}$$

$$\mathbf{W}-\mathbf{W_S} = \Omega(\mathbf{F}-\mathbf{F_S}) \tag{3.79}$$

can be found by solving the following optimization problem

$$\min_{\mathbf{f}} \quad G = \int_0^F \mathbf{W}^T d\mathbf{F} \tag{3.80}$$

$$s.t. \quad \mathbf{F} = \mathbf{M}^T \mathbf{f} \tag{3.81}$$

$$\mathbf{W_R} = \Omega(\mathbf{F_R}) \tag{3.82}$$

$$\mathbf{W_T} = const \text{ and/or } \mathbf{F_T} = const \tag{3.83}$$

or its equivalent dual

$$\min_{\mathbf{F}} \quad G = \int_0^F \mathbf{W}^T d\mathbf{F} \tag{3.84}$$

$$s.t. \quad \mathbf{MW} = \mathbf{0} \tag{3.85}$$

$$\mathbf{W_R} = \Omega(\mathbf{F_R}) \tag{3.86}$$

$$\mathbf{W_T} = const \text{ and/or } \mathbf{F_T} = const \tag{3.87}$$

Proof. Proof analogously to Theorem 14. □

Corollary 3. *For a process network with the sum of all resistive contents $G_{R,i}$ and cocontents $G^*_{R,i}$, the dissipation function $\sigma = \sum_{i=1}^{n_f} (G_{R,i} + G^*_{R,i}) = \sum_{i=1}^{n_f} W_{R,i} F_{R,i}$ is minimized if the contents and cocontents are minimized.*

Proof. The result follows directly from Theorem 14 and 15, and Tellegen's theorem (2.39). A proof using summation form is given in [25]. □

In the previous results, we show that process networks generally follow principles of self-optimization by minimizing potential gradients and re-directing flows along the paths of least resistance. Uniqueness of the solution of the regarded optimization problem is tightly connected with the functional relationships between flows and potential gradients, i.e., the constitutive equations or algorithms. In the following, we demonstrate, how constitutive equations and algorithms relate to the second order

conditions of the variational principle and concepts of convexity link to the stability of equilibria of the regarded process networks.

3.2.5 Flow Network Example

We continue the example of Section 2.3 to show how dynamic simulation can be used to converge a process network to a steady state solution showing a minimum in dissipation. The dynamic system given by the previous equations converges to the solution of the following optimization problem ($\frac{dV_1}{dt} = \frac{dV_2}{dt} = 0$):

$$\begin{aligned}
\min \quad & \sum_{i=1}^{4} \quad \int_0^{\Delta p_i} \dot{V}_i d(\Delta p_i) && (3.88)\\
s.t. \quad & dV_1/dt \quad = \dot{V}_1^{IN} - \dot{V}_1^{OUT} && (3.89)\\
& dV_2/dt \quad = \dot{V}_2^{IN} - \dot{V}_2^{OUT} && (3.90)\\
& \dot{V}_{T1} \quad = \dot{V}_2^{IN} + \dot{V}_2^{IN} && (3.91)\\
& \dot{V}_{T2} \quad = \dot{V}_2^{OUT} + \dot{V}_2^{OUT} && (3.92)\\
& \dot{V}_i \quad = \frac{\pi r_i^4}{8\eta L_i} \Delta p_i \; , i = 1,..,4 && (3.93)\\
\dot{V}_{T1} = \quad & const., p_{T2} = const. && (3.94)
\end{aligned}$$

Solving the optimization problem therefore corresponds to minimizing the power dissipated through viscous friction in the pipes subject to the conservation laws and boundary conditions. For each terminal, one boundary condition has to be specified which can be chosen freely ($\dot{V}_{T1} = 0.3$ m^3/s, $p_{T2} = 1.013$ bar). The parameters are given as $d = 0.5$ m and $L_1 = 2500$ m for the upper pipeline segments and $L_2 = 5000$ m for the lower segments. The tanks' cross-sectional diameter is chosen as $d_1 = d_1 = 2$ m. Fig. 3.4 shows the simulation results. We chose the initial conditions for $V_{0,1} = V_{0,2} = 25$ m^3. It is apparent that the value of the objective function as well as the flows of the dynamic simulation converge to the optimum determined through the optimization problem for arbitrary initial

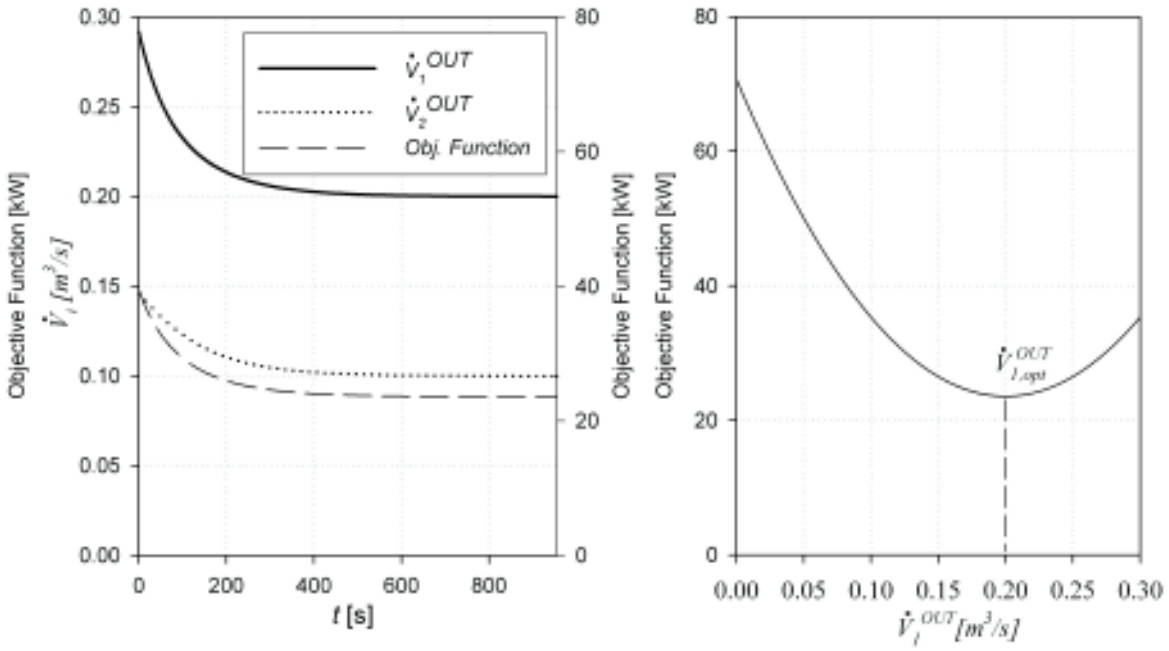

Figure 3.4: Flows between tanks and outgoing terminal T_2 and the power dissipation (objective function) as a function of time on the left. Convergence of $\dot{V}_1^{OUT} =$ to 0.2 m^3/s and $\dot{V}_2^{OUT} =$ to 0.1 m^3/s. Objective function values of $\dot{V}_1^{OUT}$ on the right.

conditions. The constant inflow $\dot{V}_{T1}$ into the network divides itself into flows through the upper segments and lower segments choosing the path of least resistance.

3.2.6 Supply Chains and the Second Law of Thermodynamics

Network theory can be applied for modeling financial, material, and service flows in business systems. Business organizations can be regarded as complex networks in which a combination of centralized and decentralized decision making aims at optimizing a business' performance [49]. Regardless of the complexity, a business' objective to maximize its profit and as a consequence its total value is often implemented through very simple decentralized management policies that lead to self-optimizing structures using key indicators such as Net Present Value or the Return on Investment [47].

We define a network of activities of a business organization according to the framework defined in Chapter 2. At the nodes of the business network, activities take place in which material, cash, or liabilities can be stored, routed, or transformed as depicted in Fig. 3.5. The connections between

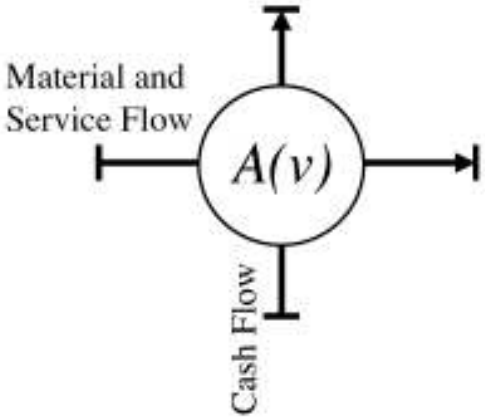

Figure 3.5: We view the business as an input-output system. There are two flows of interest. The first concerns the flow of goods and services through the system. The second concerns the flow of cash. These flows must be managed so that the business objective(s), in this case denoted by $A(v)$, where v is the state of the system, is (are) maximized.

the nodes represent material or financial flows. The terminals on the left hand side are connections to suppliers, the ones on the right hand side represent the costumers which connect the business to economic markets. For our discussion, it is convenient to define the following extensive variables when we develop an abstract framework for business decision making. These variables describe the assets

$$a = \begin{cases} a^{current} - \text{ current assets (inventory } I \text{ and cash } c) \\ a^{fixed} - \text{ fixed assets (buildings equipment)} \\ a^{other} - \text{ other assets (patents, market position)} \end{cases}$$

and liabilities

$$l = \begin{cases} l^{current} - \text{ short term liabilities (outstanding bills)} \\ l^{longterm} - \text{ long term liabilities (loans, mortgages)} \end{cases}$$

Material, service and cash flows entering and leaving a node are conserved. Forming a vector of

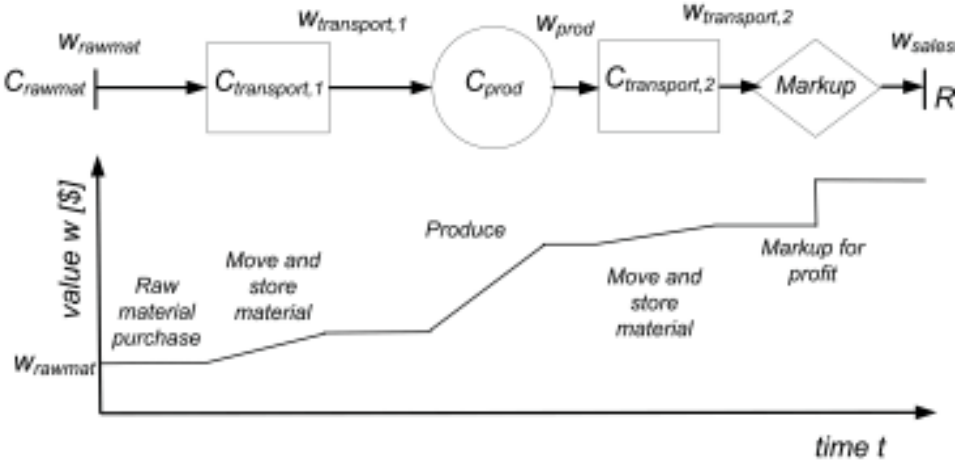

Figure 3.6: The value chain tracks how process operations add value to goods as they move through the production system. The last section includes the price markup as a value added step.

all assets $\mathbf{a}$ and liabilities $\mathbf{l}$ for each node, the inventories of assets and liabilities for all nodes $\mathbf{v}^T = (\mathbf{a_1}^T, \mathbf{l_1}^T, \mathbf{a_2}^T, \mathbf{l_2}^T, ..., \mathbf{a_{n_p}}^T, \mathbf{l_{n_p}}^T)$ determine the state of the dynamic system under consideration that the flows determine how assets and liabilities are re-allocated throughout the business organization. The dynamic system consists of input-output variables, i.e., the incoming and outgoing flows of assets and liabilities.

$$\frac{d\mathbf{v}}{dt} = \phi(\mathbf{u}, \mathbf{t}) + \mathbf{p} \tag{3.95}$$

Eq. (3.95) corresponds to Kirchhoff's current law. We now define potentials in form of prices or values w at the nodes in the network according to Chapter 2. In order to introduce potentials, we need to define an appropriate storage function for business systems. The storage function $E(v)$ is used to capture the total value of the business

$$E = A - L \tag{3.96}$$

E formally corresponds to the shareholder or owner equity (net worth) of a business. We also define

the functions value of all assets A and value of all liabilities L

$$A = \sum_{i}^{N^{a}ssets} a_i w_{a,i}, \text{value of assets [Value]} \tag{3.97}$$

$$L = \sum_{i}^{N^{a}ssets} l_i w_{l,i}, \text{ liabilities [Value]} \tag{3.98}$$

After defining an appropriate storage function for the business network, we can now derive potentials w for each node in the network through

$$w_{a,i} = \frac{\partial E}{\partial a_i} \text{ or } w_{l,i} = \frac{\partial E}{\partial l_i} \tag{3.99}$$

The company's value is then defined through the net worth or owner's/shareholder equity $E(v)$. A companies objective is to maximize its total value over time. An increase of the value can be achieved through a positive cost/profit balance of all the activities. The profit of an activity is calculated so that

$$P(t) = \int_{t}^{t+T} (R-C)ds \tag{3.100}$$

where T is the reporting period, R is the rate of income from sales, and C is the rate of cost. The difference $R-C$ is called rate of accounting earning. The activity costs include transportation, storage, manufacture (assembly), and purchase. By differentiating the expression above, we obtain the differential balance

$$\frac{dP}{dt} = R-C \tag{3.101}$$

The cost rates through transportation, manufacture, and storage corresponds to dissipative elements of our general network definition. The earnings through sales R and cost through purchase can be regarded as in/outflux of value through terminals. Analogously to the optimization problem in the last section, a business organization intends to maximize the rate of accounting earnings $R-C$ to achieve

maximum profit. This can be achieved through minimizing the total rate of cost of the network which corresponds to the optimization problem posed in the last section. A more detailed version of this section can be seen in App. A.

3.3 Second Order Conditions and Stability

The results in the previous section show how the dissipation function of a process network are embedded into an optimization problem with strong topological connections among the different network equations and a variational principle. These findings connect intensive and extensive variables through both topological and optimization related concepts of duality. One further important property apart from the topological characteristics of a process networks are the algorithms used to calculate flows from potentials. The implications of the algorithms on the process network are relevant for the second order conditions as part of the optimality principle. Here, convexity of the content and cocontent constitutes an important characteristic for stability of a process network.

Definition 9. *For a process network with inventories* $\mathbf{Z}$*, we call the steady state point* $\mathbf{Z}^*$*. A process network may have more than one steady state.*

Definition 10. *A connection* $F = \Lambda(W)$ *is said to be positive if there exists a constant* $b \geq 0$ *so that*

$$(W^1 - W^2)(F^1 - F^2) \geq \beta \left\| W^1 - W^2 \right\|^2$$

The connection is strictly positive if the inequality holds with $\beta > 0$*. A differential version of the positivity condition is given as*

$$dW\,dF \geq \beta \left\| dW \right\|^2$$

where strict positivity holds for $\beta > 0$*.*

Definition 11. *A process network is said to be dissipative [10] with respect to the supply rate* $\phi_W(\mathbf{F_T}, \mathbf{w_T})$*, if there exists a storage function* $E(\mathbf{Z})$ *so that for all* $t \geq 0$ *and all initial conditions*

$$0 \leq E(\mathbf{Z}(0)) \leq E(\mathbf{Z}(t)) + \int_0^t \phi_W(\mathbf{F_T}, \mathbf{w_T})$$

The dissipation inequality expresses the fact that the stored energy does not increase beyond supply plus initial storage.

Definition 12. *A dissipative process with input vector* $\mathbf{F_T}$ *or* $\mathbf{w_T}$ *and output vector* $\mathbf{w_T}$ *or* $\mathbf{F_T}$ *is passive [52], if there exist non-negative constants* β_i *so that the supply rate can be written*

$$\phi_W(\mathbf{F_T}, \mathbf{w_T}) = \mathbf{w_T}^T \mathbf{F_T} - \beta_1 \mathbf{F_T}^T \mathbf{F_T} - \beta_2 \mathbf{w_T}^T \mathbf{w_T}$$

Theorem 16. *A process network is passive, if the constitutive equations are positive.*

Proof. We write the conservation equations $\mathbf{AF} = \mathbf{0}$ so that

$$\frac{d\mathbf{Z}}{dt} = -\mathbf{A_R}\mathbf{F_R} - \mathbf{A_T}\mathbf{F_T} \tag{3.102}$$

Also, we have

$$\frac{dE}{dt} = \frac{\partial E}{\partial \mathbf{Z}} \frac{d\mathbf{Z}}{dt}$$

The dissipation inequality in differential form gives

$$0 \leq \frac{\partial E}{\partial \mathbf{Z}} \mathbf{A_R}\mathbf{F_R} + \frac{\partial E}{\partial \mathbf{Z}} \mathbf{A_T}\mathbf{F_T} \leq \phi_W(\mathbf{F_T}, \mathbf{w_T})$$

It follows that the process network is passive, if

$$\frac{\partial E}{\partial \mathbf{Z}} \mathbf{A_R}\mathbf{F_R} \leq \mathbf{w_T}^T \mathbf{F_T} - \beta_1 \mathbf{F_T}^T \mathbf{F_T} - \beta_2 \mathbf{w_T}^T \mathbf{w_T}$$

If we use Tellegen's theorem

$$0 \leq -\mathbf{F_R}\mathbf{W_R} - \mathbf{F_T}\mathbf{W_T} \leq \phi_W(\mathbf{F_T}, \mathbf{w_T})$$

it follows that

$$\mathbf{F_R}\mathbf{W_R} \geq \beta_1 \mathbf{F_T}^T \mathbf{F_T} + \beta_2 \mathbf{w_T}^T \mathbf{w_T} \geq 0 \tag{3.103}$$

as a condition of passivity. □

The process network is strictly input passive, if $\beta_2 > 0$ (for the potentials being the terminal input variables) and strictly output passive for $\beta_1 > 0$ (for the flows being the terminal output variables) and vice versa. If (3.103) holds, then the system is globally asymptotically stable and has a unique stationary point $\mathbf{Z}^*$. If we define a storage function such as the availability $E = (\mathbf{w}^* - \mathbf{w})^T \mathbf{Z}$ which is homogeneous and degree one, then we can show the dependence on the flow connections [25]. The definition of a storage function which is homogeneous and degree one leads to capacitive constitutive equations which are a strictly monotonous function $\mathbf{Z} = C(\mathbf{w})$ [10].

Lemma 5. *There exists a unique stable equilibrium point $\mathbf{Z}^*$ of a process network, if the corresponding optimization problem as given in Theorem 8 is globally convex.*

Proof. Starting with

$$\min_{\mathbf{w}} \quad G^* = \int_0^W \mathbf{F} d\mathbf{W} \tag{3.104}$$

$$s.t. \qquad \mathbf{W} = \mathbf{A^T w} \tag{3.105}$$

$$\mathbf{F} = \Lambda(\mathbf{W}) \tag{3.106}$$

we substitute the constraints (3.105) and (3.106) into the objective function

$$L = \int_0^w \mathbf{A}\Lambda(\mathbf{A^T w}) d\mathbf{w} \tag{3.107}$$

For a unique solution, the second order conditions have to be positive definite to ensure global convexity of the objective function. Second order conditions:

$$\frac{\partial^2 L}{\partial \mathbf{w}^2} = \mathbf{A}\frac{\partial \Lambda}{\partial \mathbf{w}}\mathbf{A}^T \tag{3.108}$$

With Theorem 8 showing the first order optimality conditions, it follows that global optimality and a unique solution is guaranteed if the Hessian matrix $\mathbf{A}\frac{\partial \Lambda}{\partial \mathbf{w}}\mathbf{A}^T$ is positive definite. □

Theorem 17. *The Hessian matrix $\mathbf{A}\frac{\partial \Lambda}{\partial \mathbf{w}}\mathbf{A}^T$ is positive definite, if $\frac{\partial \Lambda}{\partial \mathbf{w}}$ is positive definite.*

Proof. Since $\mathbf{A}$ is a full rank matrix, positive definiteness follows immediately. □

Theorem 18. *The Hessian matrix $\mathbf{A}\frac{\partial \Lambda}{\partial \mathbf{w}}\mathbf{A}^T$ is positive definite, if the constitutive equations are positive.*

Proof. Starting with the differential form of the constitutive equations for the process network

$$d\mathbf{F}^T d\mathbf{W} \geq \mathbf{0}$$

we use the constitutive equation in differential form $d\mathbf{F} = d\Lambda(\mathbf{W})$ as

$$d\Lambda(\mathbf{W})^T d\mathbf{W} \geq \mathbf{0} \tag{3.109}$$

which is equivalent to

$$d\mathbf{W}^T \frac{\partial \Lambda(\mathbf{W})}{\partial \mathbf{W}} d\mathbf{W} \geq \mathbf{0} \tag{3.110}$$

or

$$d\mathbf{w}^T \mathbf{A}\frac{\partial \Lambda}{\partial \mathbf{w}}\mathbf{A}^T d\mathbf{w} \geq \mathbf{0} \tag{3.111}$$

and the result follows. □

Lemma 6. *Suppose that we have a strictly convex potential $\sigma(F)$ so that*

$$W = \frac{\partial \sigma}{\partial F}$$

then $F = \Lambda(W)$ is positive.

Proof. See [2]. □

Theorem 19. *The optimization problem has a unique global optimum, i.e., the process network has a unique equilibrium point, if the constitutive equations are positive, i.e., the process network is passive.*

Proof. Follows immediately from Theorems 5, 16, 18, and on the basis of a convex potential from Lemma 6. □

For a given process network, we can infer the passivity property if we have strictly monotonous relationships between intensive and extensive quantities, both for the irreversible and reversible flow connections in the network. Using the optimality concepts developed in this work, it is possible to check if a particular equilibrium point of a process network is unique and stable through the corresponding dissipation function and optimization problem, i.e., it is possible to analyze stability and optimality for the process network by ensuring positivity for the individual flow connections.

3.3.1 Potential Function of a Process Network

In this section, our interest lies in the derivation of the so called potential function for the process network. Brayton and Moser [5, 6] derived a potential function for electrical circuits such that

$$\dot{Q}(\mathbf{x})\dot{\mathbf{x}} = \nabla P(\mathbf{x}) \tag{3.112}$$

where $\dot{Q}(\mathbf{x})$ is a non-singular square matrix obtained from reversible elements and $P(\mathbf{x})$ is a scalar mixed potential obtained from the irreversible constitutive equations. The mixed potential function

$$P(\mathbf{X},\mathbf{J}) = R(\mathbf{J}) - G(\mathbf{X}) + \Phi(\mathbf{J},\mathbf{X}) \tag{3.113}$$

is derived based on electrical currents $\mathbf{J}$ and voltage differences $\mathbf{X}$. The formulation given by Brayton and Moser is elegant for the analysis of non-linear analogue electrical circuits, since it treats currents and voltages as the primary variables dependent on the type of circuit element. They distinguish between inductors, capacitors, and resistors, where the matrix $\dot{Q}(\mathbf{x})$ contains all information about reversible circuit elements. Our goal is the derivation of a potential function $P(\mathbf{Z})$ based on the inventories $\mathbf{Z}$ of a process, i.e., the extensive quantities such as mass and energy as in

$$E(\dot{\mathbf{Z}}) = -\frac{\partial P(\mathbf{Z})}{\partial \mathbf{Z}} \tag{3.114}$$

We require it to contain all important information about reversible and irreversible parts of the process network in order to use it as a basis for stability analysis and the design of decentralized control systems. The function $E(\dot{\mathbf{Z}})$ is a diagonal matrix function that contains the reversible elements facilitating easier access from a control perspective than the Brayton-Moser equations. In the case of the function E($\cdot$) being an (invertible) Kirchhoff operator on $\dot{\mathbf{Z}}$ (see [42]), then the system can be transformed into a canonical system with an augmented potential function and stability and optimality follows immediately for a convex augmented potential function.

An important property of process networks is that chemical systems typically do not require the use of inductive elements. Chemical processes are generally dissipative and variations in the kinetic energy, i.e., dynamics through change of kinetic energy are usually disregarded. The extension towards complex processes involving different components including transformations, sinks, and sources requires the consistent use of inventories as primary variables to guarantee stability in the

passivity sense. We demonstrate how the concept can also be used to draw a connection to Lyapunov stability theory.

Theorem 20. *The potential function of a process network is given as*

$$P(\mathbf{Z}) = \Phi(\mathbf{Z}) + \int_0^{\mathbf{w_T}} \mathbf{F_T}^T d\mathbf{w_T}$$

where $\Phi(\mathbf{Z}) = \int_0^{\mathbf{Z}} \mathbf{A_R} \Lambda [\mathbf{A_R}^T C^{-1}(\mathbf{Z})]^T d\mathbf{Z}$

Proof. Starting with the cocontent function (3.11) and proceeding with the decomposition into terminals and resistive flows

$$G^* = \int_0^{\mathbf{W}} \mathbf{F}^T d\mathbf{W} = \int_0^{\mathbf{W_R}} \mathbf{F_R}^T d\mathbf{W^R} + \int_0^{\mathbf{w_T}} \mathbf{F_T}^T d\mathbf{w_T} \tag{3.115}$$

Using Kirchhoff's voltage law (2.27) and the resistive and capacitive constitutive equations (2.47), the result follows immediately. □

Illustrative Examples

For the example network given in Figure 2.4 the optimization problem is given as

$$\min_{\mathbf{w}} \quad G^* = \sum_{i=1}^{8} \int_0^{W_i} F_i dW_i \tag{3.116}$$

$$s.t. \quad W_1 = w_{T1} - w_1 \tag{3.117}$$

$$W_2 = w_1 - w_{T2} \tag{3.118}$$

$$W_3 = w_{T1} - w_2 \tag{3.119}$$

$$W_4 = w_2 - w_{T2} \tag{3.120}$$

$$F_i = K_i W_i,\ i = 1..4 \tag{3.121}$$

$$Z_i = C_i w_i,\ i = 1..2 \tag{3.122}$$

$$w_{T1} = \text{const},\ w_{T2} = \text{const} \tag{3.123}$$

We derive the potential function from the flow network example in Section 2.3 using the cocontent formulation as a starting point with constant potentials at the terminals:

$$G^* = \sum_{i=1}^{8} \int_0^{W_i} F_i dW_i \tag{3.124}$$

The flow connections for the dynamic nodes F_5 and F_6 vanish based on the definition of the potential function and the terminal contributions vanish due to constant potentials. We use (3.121):

$$P = \sum_{i=1}^{4} \int_0^{\Delta W_{Ri}} K_i W_{Ri} d(W_{Ri}) \tag{3.125}$$

Using Kirchhoff's voltage law and integration results into

$$\begin{aligned} P &= \frac{1}{2}K_1(w_{T1}-w_1)^2+\frac{1}{2}K_2(w_{T1}-w_2)^2 && (3.126)\\ &\quad +\frac{1}{2}K_3(w_1-w_{T2})^2+\frac{1}{2}K_4(w_2-w_{T2})^2 && (3.127)\end{aligned}$$

using the capacitive constitutive equations $w_i = \frac{Z_i}{C_i}$

$$\begin{aligned} P(Z_1,Z_2) &= \frac{1}{2}\frac{K_1+K_3}{C_1^2}Z_1^2+\frac{1}{2}\frac{K_2+K_4}{C_2^2}Z_2^2 && (3.128)\\ &\quad -\frac{1}{C_1}(K_1w_{T1}+K_3w_{T2})Z_1 && (3.129)\\ &\quad -\frac{1}{C_2}(K_2w_{T1}+K_4w_{T2})Z_2 && (3.130)\\ &\quad +\frac{1}{2}(K_1+K_2)w_{T1}^2+\frac{1}{2}(K_3+K_4)w_{T2}^2 && (3.131)\end{aligned}$$

The resulting potential function is quadratic

$$P(\mathbf{Z}) = \frac{1}{2}\mathbf{Z}^T\Phi_Z\mathbf{Z}-\mathbf{Z}^T\Phi_{Z,w_T}\mathbf{w_T}+\frac{1}{2}\mathbf{w_T}^T\Phi_{w_T}\mathbf{w_T} \quad (3.132)$$

The equilibrium points follow from the first order conditions

$$\begin{aligned} \frac{\partial P}{\partial Z_1} &= \frac{K_1+K_3}{C_1^2}Z_1-\frac{1}{C_1}(K_1w_{T1}+K_3w_{T2})=0 && (3.133)\\ \frac{\partial P}{\partial Z_2} &= \frac{K_2+K_4}{C_2^2}Z_2-\frac{1}{C_2}(K_2w_{T1}+K_4w_{T2})=0 && (3.134)\end{aligned}$$

From the second order conditions

$$\frac{\partial^2 P}{\partial Z_1^2} = \frac{K_1 + K_3}{C_1^2} > 0 \tag{3.135}$$

$$\frac{\partial^2 P}{\partial Z_2^2} = \frac{K_2 + K_4}{C_2^2} > 0 \tag{3.136}$$

$$\frac{\partial^2 P}{\partial Z_1 Z_2} = 0 \tag{3.137}$$

$$\frac{\partial^2 P}{\partial Z_2 Z_1} = 0 \tag{3.138}$$

there follows a positive definite Hessian matrix and hence a minimum. The stationary point can now be found from (3.133) and (3.134).

$$Z_1^* = C_1 \frac{K_1 w_{T1} + K_3 w_{T2}}{K_1 + K_3}, Z_2^* = C_2 \frac{K_2 w_{T1} + K_4 w_{T2}}{K_2 + K_4}$$

The second order conditions indicate global convexity and hence we find a unique stable equilibrium point for this example. In order to find the flows of the same problem through the content as functional, one has to pose the problem as

$$\max_{\mathbf{F}} \quad G^* = \sum_{i=1}^{2} \int_0^{\Delta F_{Ti}} W_i d(F_i) - \sum_{j=1}^{4} \int_0^{\Delta F_j} W_j d(F_j) \tag{3.139}$$

$$s.t. \qquad F_{T1} = F_1 + F_2 \tag{3.140}$$

$$F_{T2} = F_3 + F_4 \tag{3.141}$$

$$0 = F_1 - F_2 \tag{3.142}$$

$$0 = F_3 - F_4 \tag{3.143}$$

$$W_i = R_i F_i, \, i = 1..4 \tag{3.144}$$

$$w_{T1} = \text{const}, \, w_{T2} = \text{const} \tag{3.145}$$

The content formulation provides a "weaker" representation than the cocontent formulation if fixed potentials are used as boundary conditions. We can determine the states and the flows with the cocontent, whereas in this formulation, one can only determine the flows. The objective function is positive, since we are still minimizing the cocontent but this is done by maximizing the total power input subtracting the content.

In this problem, the terminal contributions do not vanish. We use linear resistive constitutive equations (3.144) with resistances instead of conductances:

$$P = F_{T1}w_{T1} - F_{T2}w_{T2} - \frac{1}{2}R_1F_1^2 - \frac{1}{2}R_2F_2^2 - \frac{1}{2}R_3F_3^2 - \frac{1}{2}R_4F_4^2 \tag{3.146}$$

using Kirchhoff's current law results in

$$P = (F_1 + F_3)(w_{T1} - w_{T2}) - \frac{1}{2}(R_1 + R_2)F_1^2 - \frac{1}{2}(R_3 + R_4)F_3^2 \tag{3.147}$$

We can now find the equilibrium points of the process network through the first order conditions

$$\frac{\partial P}{\partial F_1} = w_{T1} - w_{T2} - (R_1 + R_2)F_1 = 0 \tag{3.148}$$

$$\frac{\partial P}{\partial F_3} = w_{T1} - w_{T2} - (R_3 + R_4)F_3 = 0 \tag{3.149}$$

and the second order conditions

$$\frac{\partial^2 P}{\partial F_1^2} = -R_1 - R_2 < 0 \tag{3.150}$$

$$\frac{\partial^2 P}{\partial F_3^2} = -R_3 - R_4 < 0 \tag{3.151}$$

$$\frac{\partial^2 P}{\partial F_1 F_3} = 0 \tag{3.152}$$

$$\frac{\partial^2 P}{\partial Z_2 Z_4} = 0 \tag{3.153}$$

which results into a negative definite Hessian matrix and hence a maximum. We can determine the zeros of the first order conditions as

$$F_1^* = \frac{w_{T1} - w_{T2}}{R_1 + R_2}, F_3^* = \frac{w_{T1} - w_{T2}}{R_3 + R_4}$$

In the case of fixed flows at the terminals, the content formulation can be used to derive the stationary equilibrium point. In order to find the flows through the content as functional, we use

$$\min_{\mathbf{F}} \quad G = \sum_{j=1}^{4} \int_0^{\Delta F_j} W_j d(F_j) \tag{3.154}$$

$$s.t. \qquad F_{T1} = F_1 + F_2 \tag{3.155}$$

$$F_{T2} = F_3 + F_4 \tag{3.156}$$

$$0 = F_1 - F_2 \tag{3.157}$$

$$0 = F_3 - F_4 \tag{3.158}$$

$$W_i = R_i F_i, \, i = 1..4 \tag{3.159}$$

$$F_{T1} = F_{T2} = \text{const}, \tag{3.160}$$

Here, the terminal flows are fixed and balanced such that the sum of all terminal flows has to be zero in order to allow equilibrium and stability.

Similarly, as with the previous example, we can only determine the flows but not the states, such that the content formulation is considered weaker than the cocontent formulation that allows the calculation of the states.

$$P = \frac{1}{2} R_1 F_1^2 + \frac{1}{2} R_2 F_2^2 + \frac{1}{2} R_3 F_3^2 + \frac{1}{2} R_4 F_4^2 \tag{3.161}$$

using Kirchhoff's current law results into

$$P = \frac{1}{2} R_1 F_1^2 + \frac{1}{2} R_2 (F_{T1} - F_1)^2 + \frac{1}{2} R_3 F_3^2 + \frac{1}{2} R_4 (F_{T2} - F_3)^2 \tag{3.162}$$

We can now find the equilibrium points of the process network through the first order conditions

$$\frac{\partial P}{\partial F_1} = R_1 F_1 - R_2(F_{T1} - F_1) = 0 \tag{3.163}$$

$$\frac{\partial P}{\partial F_3} = R_3 F_3 - R_4(F_{T2} - F_3) = 0 \tag{3.164}$$

and the second order conditions

$$\frac{\partial^2 P}{\partial F_1^2} = R_1 + R_2 > 0 \tag{3.165}$$

$$\frac{\partial^2 P}{\partial F_3^2} = R_3 + R_4 > 0 \tag{3.166}$$

$$\frac{\partial^2 P}{\partial F_1 F_3} = 0 \tag{3.167}$$

$$\frac{\partial^2 P}{\partial Z_2 Z_4} = 0 \tag{3.168}$$

which gives a positive definite Hessian matrix and hence a minimum. We can determine the zeros of the first order conditions as

$$F_1^* = F_{T1}\frac{R_2}{R_1 + R_2}, F_3^* = F_{T2}\frac{R_3}{R_3 + R_4}$$

3.3.2 Lyapunov stability

The potential function is a direct measure for the dissipation as a function of the state. Based on the cocontent and content, we can connect the potential function directly to Lyapunov stability. The cocontent can be used as a starting point to find a Lyapunov candidate function, if a candidate equilibrium point is known.

Definition 13. *Consider an autonomous nonlinear dynamical system* $\dot{\mathbf{x}} = f(\mathbf{x})$ *then we can consider a function* $V(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$ *such that* $V(\mathbf{x}) \geq 0$ *and* $\frac{dV(\mathbf{x})}{dt} < 0$ *if* $|\mathbf{x}| \neq \mathbf{0}$ *a Lyapunov candidate function*

and the systems is stable in the sense of Lyapunov.

Theorem 21. *The potential function* $P(\mathbf{Z}) = \Phi(\mathbf{Z}) + \int_0^{\mathbf{w_T}} \mathbf{F_T}^T d\mathbf{w_T}$ *can be transformed into a Lyapunov function for a coordinate transformation* $\bar{\mathbf{Z}} = \mathbf{Z} - \mathbf{Z}^*$.

Proof. The starting point of the Lyapunov candidate function is given as the network cocontent function with deviation variables from the equilibrium point $\bar{\mathbf{Z}} = \mathbf{Z} - \mathbf{Z}^*$:

$$V(\bar{\mathbf{Z}}) = \int_0^{\bar{\mathbf{W}}(\bar{\mathbf{Z}})} \bar{\mathbf{F}}(\bar{\mathbf{Z}})^T d\bar{\mathbf{W}}(\bar{\mathbf{Z}}) \tag{3.169}$$

where $\bar{\mathbf{F}} = \mathbf{F} - \mathbf{F}^*$ and $\bar{\mathbf{W}} = \mathbf{W} - \mathbf{W}^*$.

$$V(\bar{\mathbf{Z}}) = \int_0^{\bar{\mathbf{Z}}} \mathbf{A_R} \Lambda [\mathbf{A_R}^T \mathbf{C}(\bar{\mathbf{Z}})^{-1}]^T d\bar{\mathbf{Z}} \tag{3.170}$$

The terminal contributions vanish since either the potentials or flows are fixed and hence $\int_0^{\bar{\mathbf{w}}_\mathbf{T}} \mathbf{F_T} d\bar{\mathbf{w}}_\mathbf{T} = 0$. If there exists an equilibrium point $\mathbf{Z}^*$ then there always exists a coordinate transformation $\bar{\mathbf{Z}} = \mathbf{Z} - \mathbf{Z}^*$ such that the equilibrium point of the new coordinate lies in the origin $\bar{\mathbf{Z}} = \mathbf{0}$. It follows immediately from the cocontent formulation that $V(\bar{\mathbf{Z}}) = 0$ if $\bar{\mathbf{Z}} = \mathbf{0}$.

To show if the candidate function is indeed a Lyapunov function for the system, it needs to be proven that

$$V(\bar{\mathbf{Z}}) > \mathbf{0}, \text{for } \left|\bar{\mathbf{Z}}\right| \neq \mathbf{0} \tag{3.171}$$

and

$$\frac{dV(\bar{\mathbf{Z}})}{dt} = \mathbf{A_R} \Lambda [\mathbf{A_R}^T C^{-1}(\bar{\mathbf{Z}})]^T \frac{d\bar{\mathbf{Z}}}{dt} < 0, \text{for } \left|\bar{\mathbf{Z}}\right| \neq \mathbf{0}$$

which results in

$$\frac{dV(\bar{\mathbf{Z}})}{dt} = \frac{\partial P(\bar{\mathbf{Z}})}{\partial \bar{\mathbf{Z}}}^T \frac{d\bar{\mathbf{Z}}}{dt}$$

since per definition of the potential function, we have $\mathbf{C}(\dot{\mathbf{Z}}) = -\frac{\partial P(\mathbf{Z})}{\partial \mathbf{Z}}$, it follows that

$$\frac{dV(\bar{\mathbf{Z}})}{dt} = -\dot{\mathbf{Z}}^T \frac{\partial \mathbf{w}}{\partial \mathbf{Z}} \dot{\mathbf{Z}} < 0$$

Since $V(\bar{\mathbf{Z}}) > \mathbf{0}$ due to the positivity of the cocontent, monotonicity and invertibility of the function $\mathbf{C} = \frac{\partial \mathbf{Z}}{\partial \mathbf{w}}$ lead to stability. □

An example of Lyapunov stability for the general linear case with linear constitutive equations is given in App. C.1.

Example 3. *Lyapunov stability of 2-node serial-parallel network:*

The potential function of the 2-node serial-parallel network from Example 2.3 is given as

$$\begin{aligned} P(Z_1, Z_2) &= \frac{1}{2}\frac{K_1 + K_3}{C_1^2} Z_1^2 + \frac{1}{2}\frac{K_2 + K_4}{C_2^2} Z_2^2 && (3.172) \\ &\quad -\frac{1}{C_1}(K_1 w_{T1} + K_3 w_{T2}) Z_1 && (3.173) \\ &\quad -\frac{1}{C_2}(K_2 w_{T1} + K_4 w_{T2}) Z_2 && (3.174) \\ &\quad +\frac{1}{2}(K_1 + K_2) w_{T1}^2 + \frac{1}{2}(K_3 + K_4) w_{T2}^2 && (3.175) \end{aligned}$$

In deviation variables, all terminal contributions vanish, since $\bar{w}_{T1,2} = 0$ and we have:

$$\begin{aligned} V(\bar{Z}_1, \bar{Z}_2) &= \frac{1}{2}\frac{K_1 + K_3}{C_1^2} \bar{Z}_1^2 + \frac{1}{2}\frac{K_2 + K_4}{C_2^2} \bar{Z}_2^2 \geq 0 && (3.176) \\ \frac{dV}{dt} &= -\frac{1}{C_1}\left(\frac{d\bar{Z}_1}{dt}\right)^2 - \frac{1}{C_2}\left(\frac{d\bar{Z}_2}{dt}\right)^2 < 0 && (3.177) \end{aligned}$$

The conditions for Lyapunov stability follow.

3.4 Dynamics

3.4.1 Dynamics and the Variational Principle of Process Networks

It is straightforward to show that a variational principle based on the first order representation of a process network does not follow immediately due to the asymmetry of the time derivative. A linear process system is used for clarity of the derivation which can be extended to a strictly passive process network. We split the cocontent functional into the three terms for storage, dissipation, and terminal contribution

$$J = \int_0^T G^* dt = \int_0^T \left(\int_0^{W_R} \mathbf{F_R}^T d\mathbf{W_R} + \int_0^{\mathbf{w}} \frac{d\mathbf{Z}}{dt}^T d\mathbf{w_C} + \int_0^{\mathbf{w_T}} \mathbf{F_T}^T d\mathbf{w_T} \right) dt \tag{3.178}$$

and substituting the constraints of the optimization problem into the functional (3.178), we have

$$\begin{aligned} J = \int_0^T G^* dt &= \int_0^T \frac{1}{2} \mathbf{Z}^T \mathbf{C}^{-1} \mathbf{A_R} \mathbf{K} \mathbf{A_R}^T \mathbf{C} \mathbf{Z} \\ &+ \frac{1}{2} \mathbf{w_T}^T \mathbf{A_R} \mathbf{K} \mathbf{A_R}^T \mathbf{w_T} \\ &+ \mathbf{w_T}^T \mathbf{A_R} \mathbf{K} \mathbf{A_R}^T \mathbf{C} \mathbf{Z} \\ &+ \int_0^{\mathbf{Z}} \frac{d\mathbf{Z}}{dt}^T \mathbf{C}^{-1} d\mathbf{Z} + \int_0^{\mathbf{w_T}} \mathbf{F_T}^T d\mathbf{w_T} dt \end{aligned} \tag{3.179}$$

Using deviation variables around a steady state $\bar{\mathbf{Z}} = \mathbf{Z} - \mathbf{Z}^*$, the terminal contributions vanish and the functional (3.179) transforms into

$$J = \int_0^T G^* dt = \int_0^T \left(\frac{1}{2} \bar{\mathbf{Z}}^T \Phi \bar{\mathbf{Z}} + \int_0^{\bar{\mathbf{Z}}} \frac{d\bar{\mathbf{Z}}}{dt}^T \mathbf{C}^{-1} d\bar{\mathbf{Z}} \right) dt \tag{3.180}$$

where $\Phi = \mathbf{C}^{-1} \mathbf{A_R} \mathbf{K} \mathbf{A_R}^T \mathbf{C}$. We define the Lagrangean function as

$$\mathcal{L}(\bar{\mathbf{Z}}, \dot{\bar{\mathbf{Z}}}) = \frac{1}{2} \bar{\mathbf{Z}}^T \Phi \bar{\mathbf{Z}} + \int_0^{\bar{\mathbf{Z}}} \frac{d\bar{\mathbf{Z}}}{dt}^T \mathbf{C}^{-1} d\bar{\mathbf{Z}}$$

The trajectory of the process network is given by the solution to the Euler-Lagrange equations:

$$\frac{\partial \mathcal{L}}{\partial \bar{\mathbf{Z}}} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\bar{\mathbf{Z}}}}\right) = \mathbf{0} \tag{3.181}$$

It follows that

$$\frac{\partial \mathcal{L}}{\partial \bar{\mathbf{Z}}} = \Phi \bar{\mathbf{Z}} + \mathbf{C}^{-1}\frac{d\bar{\mathbf{Z}}}{dt} = \mathbf{0} \tag{3.182}$$

and

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\bar{\mathbf{Z}}}}\right) = \mathbf{C}^{-1}\frac{d\bar{\mathbf{Z}}}{dt} \tag{3.183}$$

hence, it follows that

$$\mathbf{Z} = \mathbf{Z}^* \tag{3.184}$$

Omitting a set of constraints for the dynamic problem results in the steady state solution for the dynamic case, since the system immediately changes from the initial condition to the final state. Based on variational calculus, this instantaneous step change at time $t = 0$ from the initial condition $\mathbf{Z}(0)$ to the final state $\mathbf{Z}^*$ for all $t > 0$ could be proven using fractional calculus, i.e., pseudo-differential operators to create symmetry between an arbitrary test function and the derivative of the differential equations [26]. Since our interest lies in finding a variational principle that properly includes the time derivative, we proceed in testing a formulation of the process network that contains a symmetric time derivative.

3.4.2 Variational Principle of the Second Order Process Network

A variational principle can be developed on the idea of using the second order differential equations describing the process network, since it circumvents the asymmetry of the first order time derivative.

Theorem 22. *If there exists a potential function $P(\mathbf{Z})$ of a process network with a stable equilibrium*

point $\mathbf{Z}^*$*, then there is a variational principle given through the minimizer*

$$\min_{\mathbf{Z}} = \frac{1}{2}\int_0^T (\mathbf{Q}^T\mathbf{K}\mathbf{Q} + \dot{\mathbf{Z}}^T\mathbf{C}^{-1}\dot{\mathbf{Z}})dt \tag{3.185}$$

where $\mathbf{Q}(\mathbf{Z}) = -\frac{\partial P(\mathbf{Z})}{\partial \mathbf{Z}}$.

Proof. We begin with the definition of the potential function

$$\mathbf{E}(\dot{\mathbf{Z}}) = -\frac{\partial P(\mathbf{Z})}{\partial \mathbf{Z}} \tag{3.186}$$

We introduce the matrix function $\mathbf{Q}(\mathbf{Z}) = -\frac{\partial P(\mathbf{Z})}{\partial \mathbf{Z}}$ and differentiate (3.186) in t which results in

$$\frac{\partial \mathbf{E}}{\partial \dot{\mathbf{Z}}}\frac{d^2\mathbf{Z}}{dt^2} = \frac{\partial \mathbf{Q}}{\partial \mathbf{Z}}\frac{d\mathbf{Z}}{dt} \tag{3.187}$$

we assume linearity in $\dot{\mathbf{Z}}$ for the matrix function $\mathbf{E}(\dot{\mathbf{Z}})$ as well as in $\mathbf{Z}$ for the matrix function $\mathbf{Q}(\mathbf{Z})$

$$\mathbf{C}^{-1}\frac{d^2\mathbf{Z}}{dt^2} = \mathbf{K}\mathbf{Q} \tag{3.188}$$

Multiplying by a test function $\mathbf{v}$ with $\mathbf{v}(0) = \mathbf{v}(T) = \mathbf{0}$ and integrating between $t = 0$ and $t = T$

$$\int_0^T \left(-\mathbf{v}^T\mathbf{C}^{-1}\frac{d^2\mathbf{Z}}{dt^2} + \mathbf{v}^T\mathbf{K}\mathbf{Q}\right)dt = 0 \tag{3.189}$$

integrating by parts on the first term of the integral

$$\int_0^T \left(\frac{d\mathbf{v}}{dt}^T\mathbf{C}^{-1}\frac{d\mathbf{Z}}{dt} + \mathbf{v}^T\mathbf{K}\mathbf{Q}\right)dt = 0 \tag{3.190}$$

we define the symmetric bilinear map $a(\cdot,\cdot)$ by

$$a(u,v) = \frac{du}{dt}\frac{dv}{dt} + uv \tag{3.191}$$

applying the Babuska-Lax-Milgram theorem [28], the uniqueness of the weak solution follows and we obtain

$$\min_{\mathbf{Z}} = \int_0^T \frac{1}{2} a(\mathbf{Z},\mathbf{Z})dt \tag{3.192}$$

which is

$$\min_{\mathbf{Z}} = \frac{1}{2}\int_0^T (\mathbf{Q}^T\mathbf{K}\mathbf{Q} + \dot{\mathbf{Z}}^T\mathbf{C}^{-1}\dot{\mathbf{Z}})dt \tag{3.193}$$

The Euler-Lagrange equations for the functional $F(\mathbf{Z},\dot{\mathbf{Z}},t)$ are

$$\frac{\partial F}{\partial \mathbf{Z}} - \frac{d}{dt}\frac{\partial F}{\partial \dot{\mathbf{Z}}} = \mathbf{0} \tag{3.194}$$

resulting in

$$\mathbf{C}^{-1}\frac{d^2\mathbf{Z}}{dt^2} = \mathbf{K}\mathbf{Q} \tag{3.195}$$

Integration in time and choosing the proper initial and final conditions gives

$$\mathbf{E}(\dot{\mathbf{Z}}) = \mathbf{Q}(\mathbf{Z}) \tag{3.196}$$

with $Q(\mathbf{Z}) = -\frac{\partial P(\mathbf{Z})}{\partial \mathbf{Z}}$, the result follows. □

The use of the second derivative implies that there exist more solutions for the variational problem than if we only used the first order differential equation as a starting point. Consequently, we need to ensure proper choice of initial conditions for the second order system to guarantee consistency with the first order system.

The dynamics of the process network in this framework consist of two contributions which are

equally important for the dynamic behavior of the system. The framework allows the separation of the irreversible or dissipative and the reversible or storage-type connections. We can write the functional as

$$G^*(\mathbf{Z},\dot{\mathbf{Z}}) = \int_0^T (\Sigma(\mathbf{Z}) + \Gamma(\dot{\mathbf{Z}}))dt \tag{3.197}$$

where $\Sigma(\mathbf{Z})$ is dissipation related and $\Gamma(\dot{\mathbf{Z}})$ is the storage related function. The Euler-Lagrange equations lead to the differential equations that describe the system. The dynamic behavior on a trajectory is determined by the gradients induced through the dissipation function Σ and the process network's inertial force function Γ. We observe a natural "trade-off" between the reversible and irreversible changes in the system which are both minimized, i.e., Σ is minimized as to reach a state of maximum entropy (or minimum entropy dissipation) and Γ to minimize the forces through change of inertia of the inventories.

3.4.3 Feedback between State and Control Variables: Linear Quadratic Regulator

We define a linear quadratic problem known as the linear quadratic regulator (LQR) to show how the variational principles are related to a simple optimal control problem. We relate process networks to the common definition of the LQR.

Definition 14. *For a continuous-time linear system described by*

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u} \tag{3.198}$$

with a quadratic cost function defined as

$$J = \int_0^\infty \left(\mathbf{x}^T\mathbf{Q}\mathbf{x} + \mathbf{u}^T\mathbf{R}\mathbf{u}\right) dt \tag{3.199}$$

the feedback control law that minimizes the value of the cost is $\mathbf{u} = -\mathbf{Kx}$*, where* $\mathbf{K}$ *is given by* $\mathbf{K} = \mathbf{R}^{-1}\mathbf{B}^T\mathbf{P}$*, and* $\mathbf{P}$ *is found by solving the Riccati equation.*

$$\mathbf{A}^T\mathbf{P} + \mathbf{PA} - \mathbf{PBR}^{-1}\mathbf{B}^T\mathbf{P} + \mathbf{Q} = \mathbf{0} \tag{3.200}$$

Theorem 23. *Consider a process network with linear resistive constitutive equations* $\mathbf{F_R} = \Lambda(\mathbf{W_R})$*, linear capacitive constitutive equations* $\mathbf{Z} = \mathbf{C}(\mathbf{w})$ *and boundary conditions for each terminal as well as the conservation laws. The process network can be described as a linear quadratic regulator (LQR).*

Proof. Starting with

$$J = \int_0^\infty \left(\frac{1}{2}\bar{\mathbf{F}}_\mathbf{R}^T\mathbf{K}^{-1}\bar{\mathbf{F}}_\mathbf{R} + \dot{\bar{\mathbf{Z}}}^T\mathbf{C}^{-1}\dot{\bar{\mathbf{Z}}} \right) dt \tag{3.201}$$

and the optimization problem follows as

$$\min_{\mathbf{F_R}} \quad G^* = \int_0^\infty (\tfrac{1}{2}\bar{\mathbf{F}}_\mathbf{R}^T\mathbf{K}^{-1}\bar{\mathbf{F}}_\mathbf{R} + \dot{\bar{\mathbf{Z}}}^T\mathbf{C}^{-1}\dot{\bar{\mathbf{Z}}})dt \tag{3.202}$$

$$s.t. \qquad \frac{d\bar{\mathbf{Z}}}{dt} = -\mathbf{A_R}\bar{\mathbf{F}}_\mathbf{R} \tag{3.203}$$

Using the theory for the LQR, we derive through variational calculus

$$\dot{\mathbf{Z}} = -\mathbf{A_R}\bar{\mathbf{F}}_\mathbf{R} \tag{3.204}$$

$$\dot{\lambda} = -\mathbf{C}^{-1}\dot{\bar{\mathbf{Z}}} \tag{3.205}$$

$$\mathbf{K}^{-1}\bar{\mathbf{F}}_\mathbf{R} - \mathbf{A_R}^T\lambda = 0 \tag{3.206}$$

Combining the last two equations, we determine the feedback law between $\mathbf{Z}$ and $\mathbf{F_R}$ as $\mathbf{F_R} =$

$\mathbf{K}^{-1}\mathbf{A}_R^T\mathbf{C}^{-\mathbf{1}}\mathbf{Z}$. Using all three equations, we have

$$\frac{d\mathbf{Z}}{dt} = -\mathbf{C}\Phi(\mathbf{Z}-\mathbf{Z}^*)$$

and the result follows. □

The state (3.204) and co-state equations (3.205) as well as the set of resistive constitutive equations (3.206) or in LQR terms stationary equations are recovered for the particular problem. Eq. (3.206), the resistive constitutive equations, allow the derivation of the Lagrange multipliers as $\lambda = \mathbf{w}$, the potentials. The result is not surprising due to the duality of potentials and flows, see Section 3.2. Usually, the solution of the continuous LQR is given through the continuous Riccati equation which in this case degenerates to a trivial solution for the matrix $P = C^{-1}$. Eq. (3.205) recovers the capacitive constitutive equations in the differential form and (3.204) follows as the system of differential equations.

3.4.4 Variational Problem with Kirchhoff Laws as Inequality Constraint

This section discusses the initial idea given in Section 3.4.1, in which a set of Kirchhoff laws is omitted and replaced by the dissipation function in the functional. As can be seen, the objective function correctly models the driving force in the dynamic case, but the lack of one set of topological constraints leads to the immediate jump from the initial state to the equilibrium state, i.e., the state of minimum entropy production. In this section, we discuss, how the removed set of Kirchhoff laws can function as an inequality constraint rather than an equality constraint.

The macroscopic properties and therefrom following constitutive equations and parameters are averaged quantities formally representing a statistical function of the micro-states and their dynamics. These macroscopic equations describe limits for the rate of change of the system and reflect inertial forces that limit the rate of change of the microscopic dynamics. Open systems not only seek to

converge to a state of maximum entropy, but also show a tendency to converge to the favorable state as quickly as possible [23]. In the case of irreversible thermodynamic systems with persistent gradients, it translates to finding the trajectory that maximizes the change in entropy production in order to reach minimum entropy production in minimum time. Since the gradient of entropy production is subject to mass conservation, energy conservation and the inertial forces encountered on the microscopic levels, the system naturally seeks to optimize the transient process by operating with active constraints, i.e., limitations described by macroscopic equations in form of inequality constraints become active and are effectively treatable as equality constraints. Generally, the change of entropy in a thermodynamic process in a particular volume can be written as

$$\frac{\partial S}{\partial t} = -\frac{\partial}{\partial x} J_S + \sigma_S \tag{3.207}$$

where S is the entropy density per unit volume, J_S is the entropy flux and σ_S the entropy production per unit of volume. The entropy source/sink term can be given as the product of conjugate fluxes and thermodynamic forces. From the network perspective, we can regard the entropy balance as

$$\frac{dS}{dt} = \frac{1}{T}\frac{dU}{dt} \tag{3.208}$$

where $\frac{dU}{dt}$ follows directly from the power balance or Tellegen's theorem, see (2.39) in Chapter 2. We regard the exo-system as constant in its intensive variables, i.e., heat transfer from the process system to the exo-system does not increase the temperature of the exo-system, since the process system is considered small compared to the exo-system. As a result, we regard the dissipated heat as irreversible change of the entropy $\frac{dS_{irr}}{dt}$. For the process network subsystem, the production of heat through dissipation can only increase the entropy of the exo-system, and simultaneously increase the total change of entropy $dS \geq 0$ for the entire closed system consisting of exo-system and process network. Consequently, the process system's dissipation function can be seen as an entropy sink of

the process system and we have

$$\frac{dS_{irr}}{dt} = -\frac{1}{T}\left(\int_0^{W_R} \mathbf{F_R}^T d\mathbf{W_R} + \int_0^{F_R} \mathbf{W_R}^T d\mathbf{F_R}\right) \tag{3.209}$$

The process system maximizes the increase in total entropy and hence minimizes the dissipation function

$$\max \int_0^T T\frac{dS_{irr}}{dt} \quad = \min \int_0^T \int_0^{W_R} \mathbf{F_R}^T d\mathbf{W_R} + \int_0^{F_R} \mathbf{W_R}^T d\mathbf{F_R} \tag{3.210}$$

$$s.t. \qquad \text{inventory conservation} \tag{3.211}$$

$$\text{energy conservation} \tag{3.212}$$

$$\text{constitutive equations} \tag{3.213}$$

$$\text{boundary conditions} \tag{3.214}$$

A rigorous formulation of the optimization problem is case dependent, due to how boundary conditions can influence the problem. We propose a formulation of the optimization problem as

$$\min_{\mathbf{w}} \quad G^* = \int_0^T \left(\sum_{i=1}^b \int^{W_i} F_i dW_i\right) dt \tag{3.215}$$

$$s.t. \qquad \mathbf{W} = \mathbf{A^T w} \tag{3.216}$$

$$|\mathbf{AF}| \geq \mathbf{0} \tag{3.217}$$

$$\mathbf{F_R} = \mathbf{K W_R} \tag{3.218}$$

$$\mathbf{Z} = \mathbf{C w} \tag{3.219}$$

$$\mathbf{Z}(0) = \mathbf{Z_0} \tag{3.220}$$

$$\mathbf{w_T} = \text{const} \tag{3.221}$$

where Kirchhoff's current law is given as an inequality constraint. The inequality allows the sum

of flows around a node to be larger than what is suggested by conservation. Due to the tendency of the system to minimize dissipation, the flows are adjusted to be as small as possible at any state of the process system. The reduction of the flows to the minimum possible, i.e., the limit of Kirchoff's current law to be met is hence the optimal solution. The inequality can in principle be present in either of the Kirchhoff laws. A similar formulation can be given for the dual problem with constant flows at the terminals, see App. C.2. In the dual version, Kirchhoff's voltage law is given as an inequality constraint which allows the absolute value of the sum of potential differences to be greater than zero.

2-Node Flow Network Example

As a small scale example, we solve the dynamic optimization problem

$$\max_{\mathbf{F}} \quad G^* = \sum_{i=1}^{2} \int_0^{\Delta F_{Ti}} W_i d(F_i) - \sum_{j=1}^{4} \int_0^{\Delta F_j} W_j d(F_j) \tag{3.222}$$

$$s.t. \qquad F_{T1} = F_1 - F_2 \tag{3.223}$$

$$F_{T2} = F_3 - F_4 \tag{3.224}$$

$$|\tfrac{dZ_1}{dt}| \leq F_1 - F_2 \tag{3.225}$$

$$|\tfrac{dZ_2}{dt}| \leq F_3 - F_4 \tag{3.226}$$

$$W_1 = w_{T1} - w_1 \tag{3.227}$$

$$W_2 = w_1 - w_{T2} \tag{3.228}$$

$$W_3 = w_{T1} - w_2 \tag{3.229}$$

$$W_4 = w_2 - w_{T2} \tag{3.230}$$

$$F_i = K_i W_i,\ i = 1..4 \tag{3.231}$$

$$Z_i = C_i w_i,\ i = 1..2 \tag{3.232}$$

$$w_{T1} = \text{const}, w_{T2} = \text{const} \tag{3.233}$$

The problem is fully discretized into a linear quadratic program using an explicit Euler scheme, solved using GAMS, and compared to a simulation carried out in MATLAB, see Fig. 3.7. We can gain a different perspective of the problem by regarding the potential field given through the dissipation function. In principle, the dissipation function constraints the state of the system as a surface and limits the rate of change with which the process systems state can converge to the steady state, i.e., the optimum. The system choses the path of steepest descent as can be seen for the simple network example in Fig. 3.8. We analyzed the same flow network for a nonlinear case, where cubic constitutive equations were given for the flows F_2 and F_4

$$F_2 = AW_2^3 + BW_2^2 + CW_2 \tag{3.234}$$

$$F_4 = AW_4^3 + BW_4^2 + CW_4 \tag{3.235}$$

with constant coefficients $A = 1.6$, $B = -5.4$, and $C = -58.8$ for the cubic constitutive equations. The surface for the case with cubic constitutive equations, shows a number of local minima, to which the trajectories converge, as well as saddle points and a local maximum, see Fig. 3.9. The example shows how nonlinear functions lead to local minima of entropy production.

A formal proof of the results given from simulation has not been found as of now. A fully

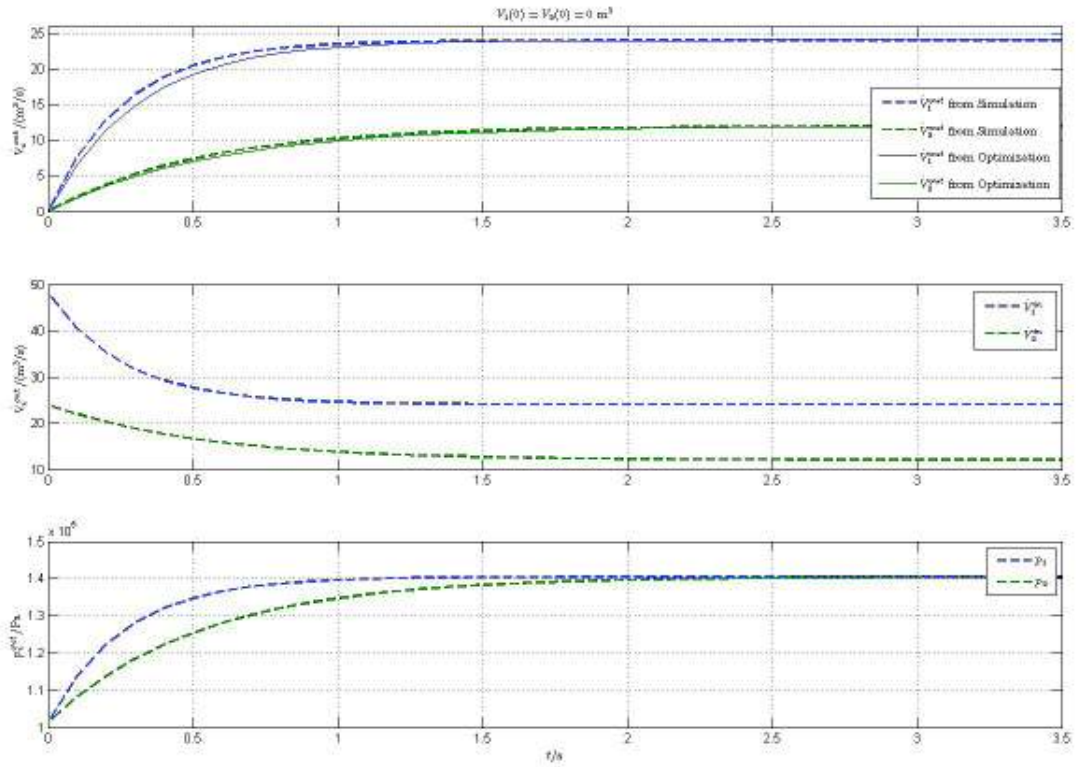

Figure 3.7: Flows of optimization problem solved in GAMS versus simulation solved in MATLAB.

discretized (explicit Euler scheme) problem can be formulated as

$$\min_{\mathbf{w}} \quad \Sigma_{k=0}^{T}\left(\Sigma_{i=1}^{b}\int^{W_i^k} F_i^k dW_i^k\right) \tag{3.236}$$

$$s.t. \quad \mathbf{W}^k = \mathbf{A^T}\mathbf{w}^k,\ k = 0..T \tag{3.237}$$

$$|\tfrac{1}{\Delta T}(\mathbf{Z}^{k+1} - \mathbf{Z}^k)| \geq -\mathbf{A_R}{\mathbf{F_R}}^k - \mathbf{A_T}{\mathbf{F_T}}^k \tag{3.238}$$

$${\mathbf{F_R}}^k = \mathbf{K}{\mathbf{W_R}}^k \tag{3.239}$$

$$\mathbf{Z}^k = \mathbf{C}\mathbf{w}^k \tag{3.240}$$

$$\mathbf{Z}^0 = \mathbf{Z_0} \tag{3.241}$$

$$\mathbf{w_T^k} = \text{const} \tag{3.242}$$

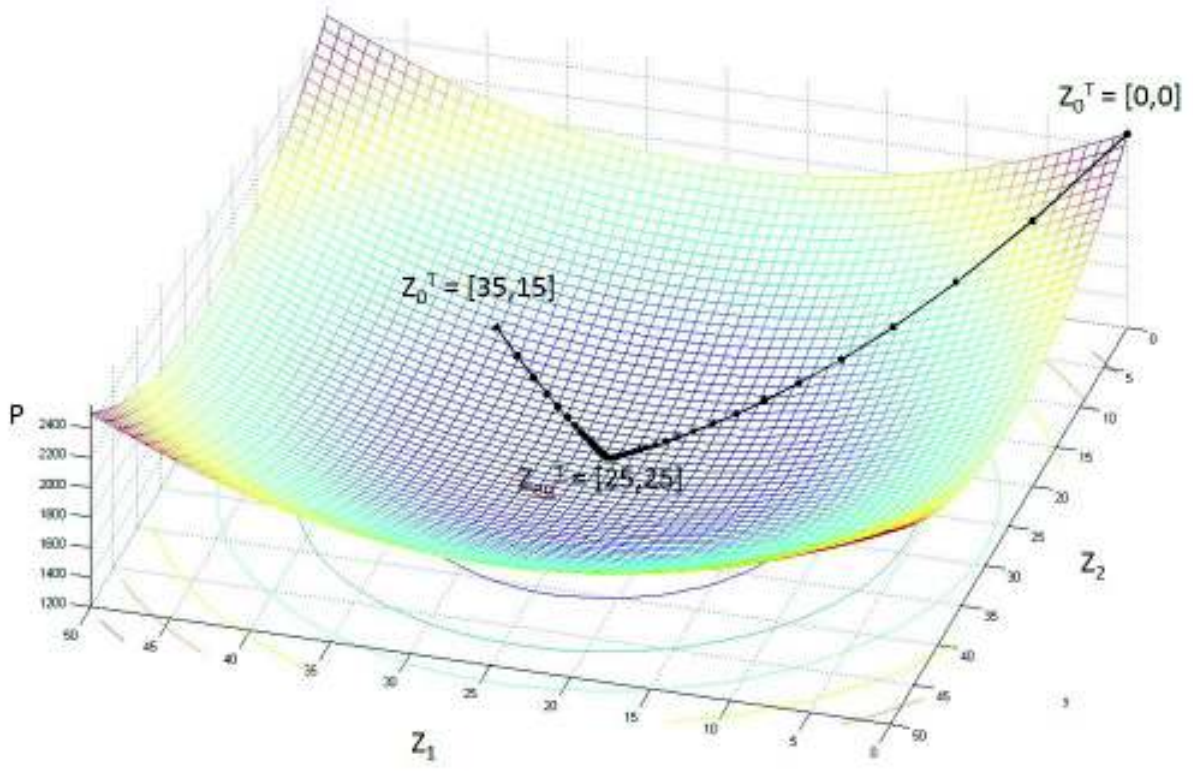

Figure 3.8: Surface of potential function with two give trajectories from initial conditions following the path of steepest descent to the minimum dissipation state.

We propose the following conjecture:

Conjecture 1. *The Karush-Kuhn-Tucker conditions given as*

$$\nabla G^{*k} + \lambda^T \nabla(\mathbf{AF})^k + \mu^T \nabla(\mathbf{W} = \mathbf{A^T w})^k = 0 \tag{3.243}$$

hold, if the Lagrangian multipliers $\lambda = \mathbf{F}$ *and* $\mu = \mathbf{w}$. *The other possible proof goes through varia-*

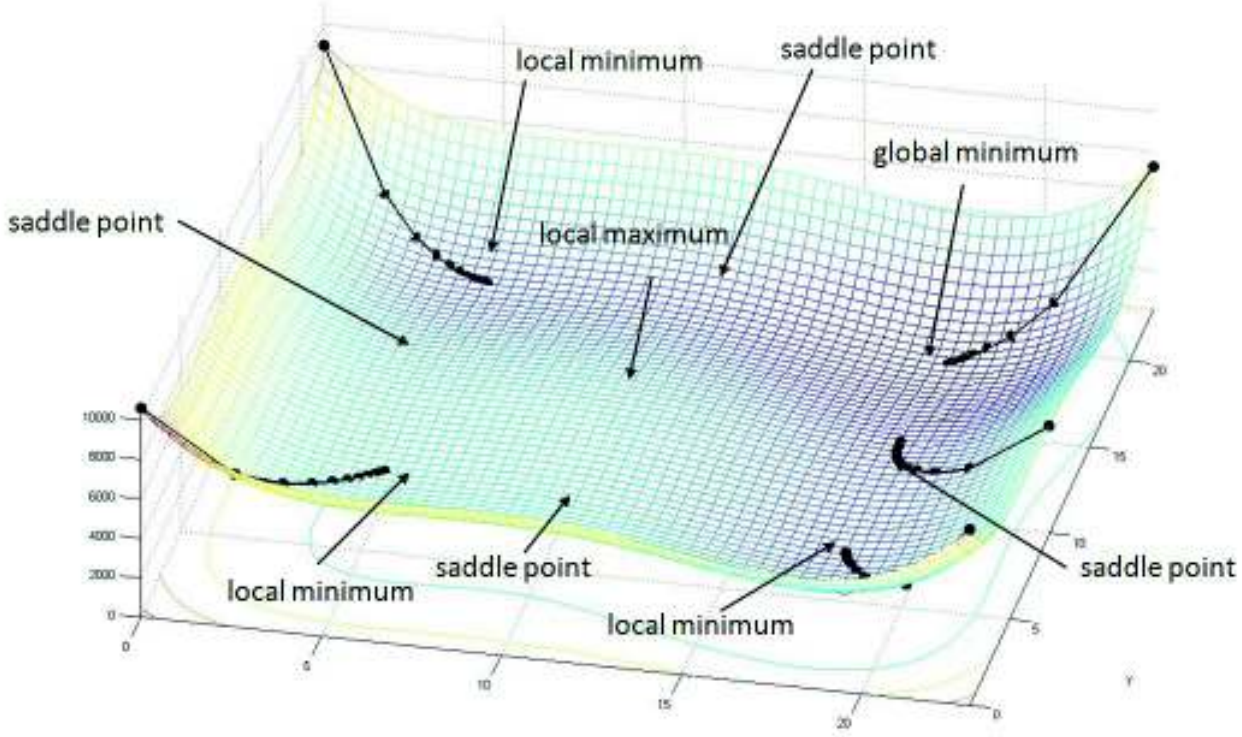

Figure 3.9: Dissipation surface for nonlinear cubic constitutive equations.

tional calculus and basically solves a path constraint optimal control problem of the form

$$\min_{\mathbf{F_R}} \quad G^*(T) + \int_0^T G^*(\mathbf{Z}(t),t)dt \tag{3.244}$$

$$s.t. \qquad |(\dot{Z})| \leq -\mathbf{A_R}\mathbf{F_R} \tag{3.245}$$

$$\mathbf{Z}(0) = \mathbf{Z_0} \tag{3.246}$$

$$\mathbf{w_T} = const \tag{3.247}$$

where

$$G^*(\mathbf{Z}(t),t) = \frac{1}{2}(\mathbf{Z}(t) - \mathbf{Z}^*)^T \Phi(\mathbf{Z}(t) - \mathbf{Z}^*)$$

and

$$\Phi(\mathbf{C},\mathbf{K}) = \mathbf{C}^{-1}\mathbf{A_R}\mathbf{K}\mathbf{A_R}^T\mathbf{C}$$

$\mathbf{Z}^* = \arg\min_Z G^*(Z(T))$ leads then to a representation of a process network trajectory identical to the corresponding system of differential equations.

3.4.5 Process Networks and the Hamilton-Jacobi-Bellman Equation

An open question from a feedback and control perspective remains for how a process network's state changes from a particular state at time t to a state $t+\Delta t$ based on the entropy production as driving force. Formally, the particular trajectory from a point in time t to $t+\Delta t$ ought to be described by a feedback policy that treats the system similarly to a Markov process, i.e., the probability distribution of the micro-states of the process network at $t+\Delta t$ are independent of the history previous to the states for $t<0$. We suppose that the process network feedback policy can be described by an equation adapted from the Hamilton-Jacobi-Bellman equation.

Conjecture 2. *Consider the following functional describing the entropy production of a process network*

$$\min_{\mathbf{F}} \sigma_S[\mathbf{Z}(T)] + \int_0^T \frac{d\sigma_S[\mathbf{F}(t),\mathbf{Z}(t)]}{dt} \tag{3.248}$$

where $\frac{d\sigma_S[\mathbf{F}(t),\mathbf{Z}(t)]}{dt}$ *is the gradient of the scalar rate function and* $\sigma_S[\mathbf{Z}(T)]$ *is the dissipation function that gives the dissipation at the final state* $\mathbf{Z}(T)$*,* $\mathbf{Z}(t)$ *is the system state vector,* $\mathbf{Z}(0)$ *is assumed given, and* $\mathbf{F}(t)$ *for* $0 \leq t \leq T$ *is the vector of flows defined as the control variables. The system is also subject to*

$$\dot{\mathbf{Z}} = f(\mathbf{Z}(t),\mathbf{F}(t)) \tag{3.249}$$

where (3.249) *is composed of the constitutive equation and the conservation law for the inventories*

Z. *For this process network, the Hamilton-Jacobi-Bellman equivalent is*

$$\dot{V}(\mathbf{Z}(t),t)+\min_{\mathbf{F}}\left\{\frac{\partial V(\mathbf{Z}(t),t)}{\partial \mathbf{Z}}^{T} f(\mathbf{Z}(t),\mathbf{F}(t))+\frac{d\sigma_S[\mathbf{F}(t),\mathbf{Z}(t)]}{dt}\right\} \tag{3.250}$$

where $V(\mathbf{Z}(t),t)$ *represents an optimal value function that is closely related to the process networks entropy.*

The feedback policy follows from Bellman's principle of optimality as

$$V(\mathbf{Z}(t),t)=\min_{\mathbf{F}}\left\{\frac{d\sigma_S[\mathbf{F},\mathbf{Z}(t)]}{dt}dt+V(\mathbf{Z}(t+dt),t+dt)\right\} \tag{3.251}$$

From (3.250), calculating the first order equations associated with the Bellman equation and applying the envelope theorem to eliminate the derivatives of the value function equations, we obtain a system of differential equations being the Euler-Lagrange equations [4]. We expect the system of differential equations to correspond to the process network equations.

Chapter 4

Decentralized Optimization and Control

"*Naturae enim non imperatur nisi parendo*."

Francis Bacon

Computer control and optimization address the problem of how to manage interaction between a complex physical network and an information system. The objective is to design an integrated network of computational devices which operates the given process network so that it follows an optimal trajectory. This task is achieved by linking signals y through algorithms with the controlled variables u, as illustrated in Fig. 4.1. The signals, y and u, represent measured outputs and control inputs. The vectors f_{ij} can be thought of as physical flows which connect one process system to other process systems or the environment.

In previous chapters, we have shown the intrinsic optimization principle found in process networks following for conservation principles and continuity. Processes and process flows tend to minimize potential gradients and naturally converge to a state of minimum dissipation. Dissipation is closely related to energy usage, i.e., there is a connection between the natural objective and eco-

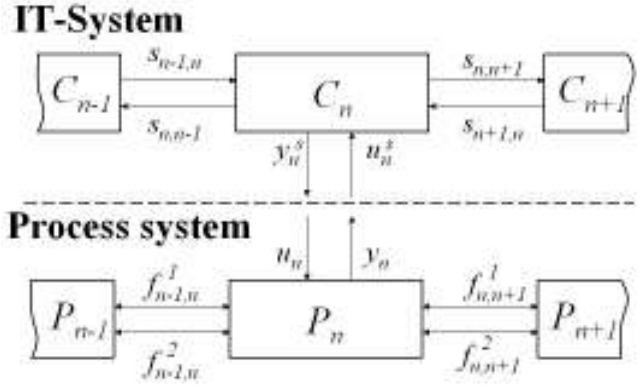

Figure 4.1: The process operator $\mathcal{P}$ maps physical flows into physical flows and measurements and actuator signals u into measurements y. In process control, we focus on the operator $G_c : u \mapsto y$ that describes how measurements and controls are related. For the modeling of process systems, we focus on the operator G_p: $r \mapsto s$ which addresses the physics but ignores the idea of measurement and control. In the figure, the arrows refer to directionality of the flows.

nomic objectives. Designing decentralized control systems often means embedding the economic objective in form of selectivity criteria into the process network's intrinsic thermodynamic characteristics. Physical connections between different parts of process networks and their contribution to the network's dynamics have to be understood and represented in the control structure design [46].

Fig. 4.2 shows a chemical plant with a decentralized control system (DCS). The physical interconnections between parts of the plant are mirrored by the controller network through information connections [55]. Control and optimization of a process network usually addresses several important objectives which are related to safety, economic performance, and stable operation in the face of disturbances [11]. We define maximization of the output of a particular product (or several products) as the primary goal of a process network. Certain transformations such as chemical reactions occur internally in the process and lead to creation of value between the entering and exiting materials and energy. The process network operates at the limits, i.e., the throughput for a fixed process network design is maximized.

During the design phase of the process network, it is important to decide which flows of the network have to be controlled and what measurements have to be taken to achieve controllability and

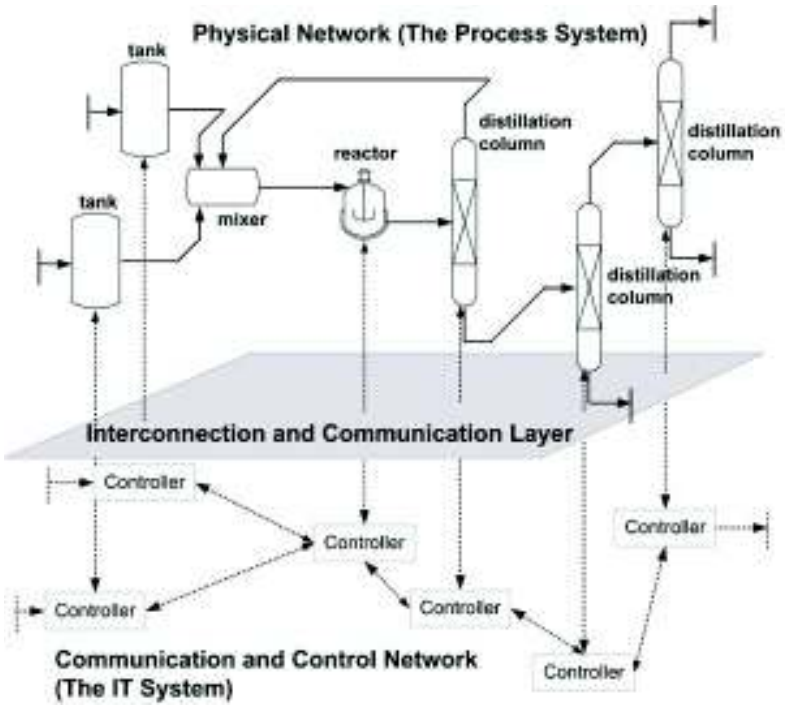

Figure 4.2: Chemical process plant with controller network.

observability. Secondly, during operation, control action almost always comes with a cost trade-off involved through loss of optimality either by reducing throughput or selectivity. In this chapter, we explain how control algorithms have to be chosen and placed in order to allow effective operation through a decentralized information network in the face of disturbances caused by the exo-system. Communication among the controllers plays as essential a role as a proper choice of feedback laws and algorithms between measurements and control variables.

4.1 Control Configuration for Inventory Control

In this section, we demonstrate, how the dynamics of the process network change under the assumption of perfect control [14]. We assume that a process network can be optimized in an ideal manner, if all inventories can be controlled perfectly. We begin with a several definitions.

Definition 15. *An inventory control strategy is said to be **direct**, if the assignment of the controllable flow $F_{K,i}$ and the inventory Z_i are incident, i.e. the flow $F_{k,i}$ either enters (supply) or leaves the node (demand).*

The concept of direct control is important, since it is related to the idea of passive systems.

Definition 16. *A process network with n_p inventories Z_i is controllable if there exists one independent directly controlled flow $F_{k,i}$ for each Z_i.*

We define an algorithm for the direct control of an inventory Z_i at node i with the controllable flow $F_{K,i}$

$$F_{K,i} = \sum F_{M,j} - f(Z_i) \tag{4.1}$$

where $F_{M,j}$ are the remaining flows incident with the node i. These flows have to be measured or related to measured quantities through models. $f(Z_i)$ is a feedback function being linear, nonlinear, or discrete in order to describe how deviations from the optimal state are handled by the flow $F_{K,i}$. A graphical illustration of the information flow for the algorithm can be seen in Fig. 4.3. An explicit

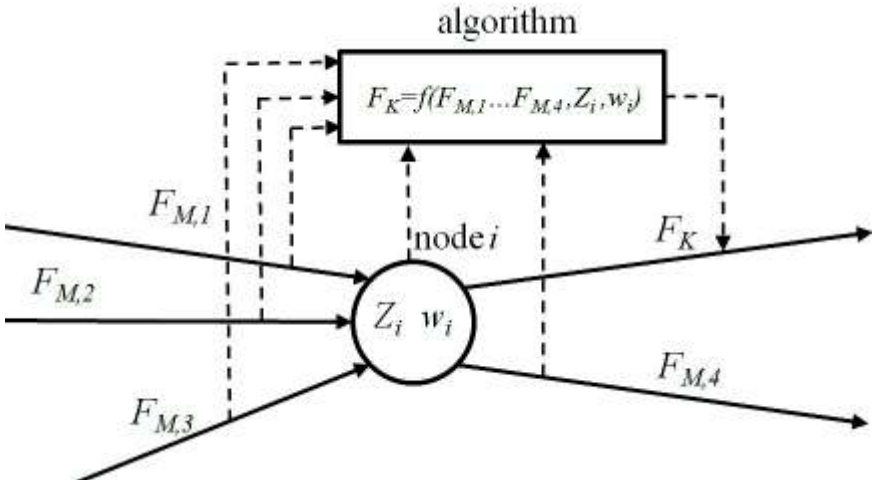

Figure 4.3: An algorithm measuring the flows $F_{M,i}$ and the potential w_i or inventory Z_i as inputs and computes the control action taken by the controlled flow F_K.

expression for the control law follows from Kirchhoff's current law as

$$\mathbf{F_K} = -\mathbf{A_K}^{-1}\mathbf{A_R}\mathbf{F_R} + \mathbf{A_K}^{-1}\Phi(\mathbf{Z}) \tag{4.2}$$

where the matrix $\mathbf{A_K}$ describes the topology of the connections between the controllable flows $\mathbf{F_K}$ and the controlled inventories $\mathbf{Z}$. A derivation of the control law is given in App. D.1. The matrix $\mathbf{A_R}$ captures the connections between the nodes and the resistive, uncontrollable flows $\mathbf{F_R}$. The matrix $\mathbf{A_K}$ is symmetric and full rank, hence invertible. Using the decentralized proportional controller as an example, we get

$$\mathbf{F_K} = -\mathbf{A_K}^{-1}\mathbf{A_R}\mathbf{F_R} + \mathbf{A_K}^{-1}\mathbf{K_C}(\mathbf{Z} - \mathbf{Z^c}) \tag{4.3}$$

The matrix $\mathbf{K_C}$ is diagonal and contains the gains of the proportional controllers and $\mathbf{Z}^c$ is the vector of setpoints for the inventory.

Theorem 24. *The potential function of a process network $P(\mathbf{Z})$ with fixed potentials at the terminals leads to the following potential function through the application of proportional controllers* (4.3) *for the controllable flows as*

$$P^c(\mathbf{Z}) = \mathbf{K_C}\mathbf{C}^{-1}\int^{\mathbf{Z}} (\mathbf{Z} - \mathbf{Z^c})^T d\mathbf{Z} \tag{4.4}$$

Proof. We begin with the optimization problem from Chapter 3, (3.19)-(3.21) determining the potential function

$$\min_{\mathbf{w}} \quad G^* = \int_0^{\mathbf{W}} \mathbf{F}^T d\mathbf{W} \tag{4.5}$$

$$s.t. \qquad \mathbf{W} = \mathbf{A}^T\mathbf{w} \tag{4.6}$$

$$\mathbf{F} = \Lambda(\mathbf{W}) \tag{4.7}$$

$$\mathbf{W_S} = \mathbf{W_T} \tag{4.8}$$

$$\mathbf{Z} = \mathbf{C}\mathbf{w} \tag{4.9}$$

We split the objective function and constraints into subsets specific to the controllable flows $\mathbf{F_K}$, resistive flows $\mathbf{F_R}$, and terminal flows $\mathbf{F_T}$

$$\min_{\mathbf{w}} \quad G^* = \int_0^{\mathbf{W_K}} \mathbf{F_K}^T d\mathbf{W_K} + \int_0^{\mathbf{W_R}} \mathbf{F_R}^T d\mathbf{W_R} + \int_0^{\mathbf{W_T}} \mathbf{F_T}^T d\mathbf{w_T} \tag{4.10}$$

$$s.t. \qquad \mathbf{W_K} = \mathbf{A_K}^T \mathbf{w} \tag{4.11}$$

$$\mathbf{W_R} = \mathbf{A_R}^T \mathbf{w} \tag{4.12}$$

$$\mathbf{W_T} = \mathbf{A_T}^T \mathbf{w_T} \tag{4.13}$$

$$\mathbf{F_K} = \Lambda_K(\mathbf{W_K}) \tag{4.14}$$

$$\mathbf{F_R} = \Lambda_K(\mathbf{W_R}) \tag{4.15}$$

$$\mathbf{w_t} = \text{const.} \tag{4.16}$$

$$\mathbf{Z} = \mathbf{C}\mathbf{w} \tag{4.17}$$

The constitutive equations for $\mathbf{F_R}$ are redundant, since we assume that their resistances are adjusted freely using the control law, given by (4.3) and added to the optimization problem as constraints. The derivatives for the potential differences follow as

$$d\mathbf{W_K} = \mathbf{A_K} d\mathbf{w} \tag{4.18}$$

$$d\mathbf{W_R} = \mathbf{A_R} d\mathbf{w} \tag{4.19}$$

$$d\mathbf{w_T} = \mathbf{0} \tag{4.20}$$

where $\mathbf{A_K}^T = \mathbf{A_K}$ since $\mathbf{A_K}$ is diagonal. The control law for $\mathbf{F_K}$ is now substituted into the objective function. The first term in (4.10) can then be written

$$\int_0^{\mathbf{W_K}} \mathbf{F_K}^T d\mathbf{W_K} = \int_0^{\mathbf{W_K}} (-\mathbf{A_K}^{-1}\mathbf{A_R}\mathbf{F_R} + \mathbf{A_K}^{-1}\mathbf{K_C}(\mathbf{Z} - \mathbf{Z^c}))^T \mathbf{A_K} d\mathbf{w} \tag{4.21}$$

hence

$$\int_0^{W_K} \mathbf{F_K}^T d\mathbf{W_K} = -\int_0^{\mathbf{w}} (\mathbf{A_R F_R})^T d\mathbf{w} + \int_0^{\mathbf{w}} \mathbf{A_K}^{-1} \mathbf{K_C} (\mathbf{Z} - \mathbf{Z^c})^T \mathbf{A_K} d\mathbf{w} \tag{4.22}$$

using the fact that $\mathbf{A_K}^{-1}\mathbf{A_K} = \mathbf{I}$. The second term in (4.10) can be written

$$\int_0^{W_K} \mathbf{F_R}^T d\mathbf{W_R} = \int_0^{\mathbf{w}} (\mathbf{A_R F_R})^T d\mathbf{w} \tag{4.23}$$

by substituting (4.22) and (4.23) into (4.10) we get

$$\min_{\mathbf{Z}} \quad P^c(\mathbf{Z}) = \textstyle\int_{\mathbf{0}}^{\mathbf{Z}} (\mathbf{Z} - \mathbf{Z^c})^T \mathbf{K_C} \mathbf{C}^{-1} d\mathbf{Z} \tag{4.24}$$

$$s.t. \qquad \mathbf{F_R} = \Lambda_K(\mathbf{W_R}) \tag{4.25}$$

and the result follows. □

Effectively, this shows that the influence of the resistive constitutive equations is removed from the potential function and dominated by the control action. The resistive constitutive equations are formally still part of the equation system although becoming redundant in determining the shape of the potential function.

Under the assumption of constraints on the controller action in form of lower and upper bounds for the controlled flows $\mathbf{F_K^{LB}} \leq \mathbf{F_K} \leq \mathbf{F_K^{UB}}$, the system returns to its original dynamics if the controlled flows hit a bound and since the control law becomes ineffective. Generally, the dynamic system described through

$$E(\dot{\mathbf{Z}}) = -\frac{\partial P(\mathbf{Z})}{\partial \mathbf{Z}} \tag{4.26}$$

with the original potential function

$$P(\mathbf{Z}) = \frac{1}{2}(\mathbf{Z} - \mathbf{Z}^*)^T \Phi (\mathbf{Z} - \mathbf{Z}^*)$$

changes into the control potential function

$$P^c(\mathbf{Z}) = \frac{1}{2}(\mathbf{Z}-\mathbf{Z}^c)^T \mathbf{K_C}\mathbf{C}^{-1}(\mathbf{Z}-\mathbf{Z}^c)$$

for the linear quadratic case. Theorem 24 shows that it is possible to change the original steady state and dynamics of the process network to a desired control potential function under certain conditions.

4.1.1 Flow Network Example

To illustrate the effect of linear control, we consider the serial-parallel network example of Chapter 2 and 3. The control configuration and algorithms are displayed in Fig. 4.4. The optimization problem

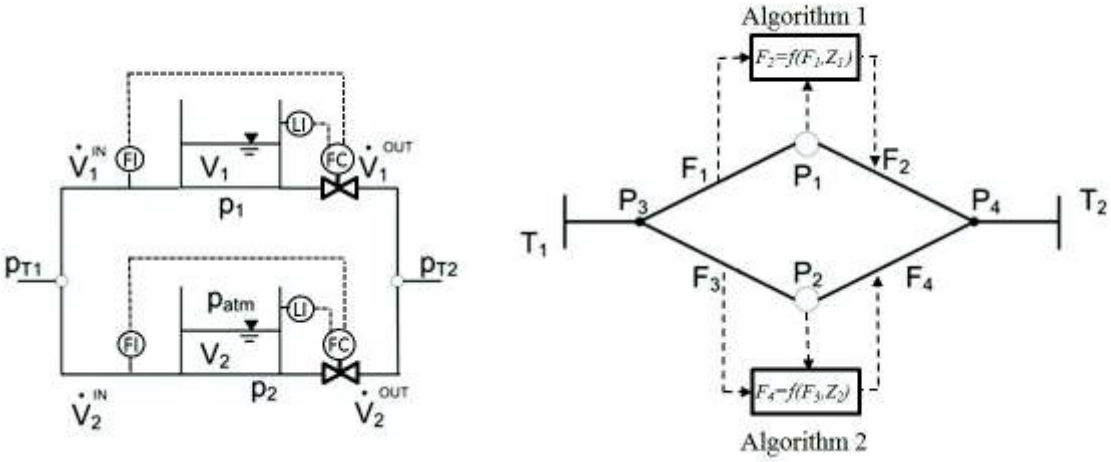

Figure 4.4: Process control configuration with two control algorithms measuring the supply flows F_1 and F_3 and the inventories Z_1 and Z_2 at the nodes and controlling the demand flows F_2 and F_4.

is now given as

$$\min_{\mathbf{w}} \quad G^* = \sum_{i=1}^{4} \int_0^{W_i} F_i dW_i \tag{4.27}$$

$$s.t. \quad W_1 = w_{T1} - w_1 \tag{4.28}$$

$$W_2 = w_1 - w_{T2} \tag{4.29}$$

$$W_3 = w_{T1} - w_2 \tag{4.30}$$

$$W_4 = w_2 - w_{T2} \tag{4.31}$$

$$F_i = K_i W_i,\ i = 1..4 \tag{4.32}$$

$$Z_i = C_i w_i,\ i = 1..2 \tag{4.33}$$

$$w_{T1} = \text{const},\ w_{T2} = \text{const} \tag{4.34}$$

The control algorithms, give two additional constraints

$$F_2 = F_1 - K_{C,1}(Z_1 - Z_1^c) \tag{4.35}$$

$$F_4 = F_3 - K_{C,2}(Z_2 - Z_2^c) \tag{4.36}$$

The potential function is derived as

$$P = \int_0^{W_1} F_1 dW_1 + \int_0^{W_2} [F_1 - K_{C,1}(Z_1 - Z_1^c)] dW_2 \tag{4.37}$$

$$+ \int_0^{W_3} F_3 dW_3 + \int_0^{W_4} [F_3 - K_{C,2}(Z_2 - Z_2^c)] dW_4 \tag{4.38}$$

Using $dW_1 = -dW_2 = -dw_1$ and $dW_3 = -dW_4 = -dw_2$ gives

$$P = \int_0^{w_1} K_{C,1}(Z_1 - Z_1^c) dw_1 + \int_0^{w_2} [K_{C,2}(Z_2 - Z_2^c)] dw_2 \tag{4.39}$$

Using the capacitive constitutive equations, the resulting potential function is quadratic

$$P(Z_1,Z_2) = \frac{1}{2}\frac{K_{C,1}}{C_1}(Z_1 - Z_1^c)^2 + \frac{1}{2}\frac{K_{C,2}}{C_2}(Z_2 - Z_2^c)^2 \tag{4.40}$$

The equilibrium points trivially follow as $Z_{1,2} = Z_{1,2}^c$ from the first order conditions. Hence, convexity and a minimum follow from the second order conditions

$$\frac{\partial^2 P}{\partial Z_1^2} = \frac{K_{C,1}}{C_1} > 0 \tag{4.41}$$

$$\frac{\partial^2 P}{\partial Z_2^2} = \frac{K_{C,2}}{C_2} > 0 \tag{4.42}$$

$$\frac{\partial^2 P}{\partial Z_1 Z_2} = 0 \tag{4.43}$$

$$\frac{\partial^2 P}{\partial Z_2 Z_1} = 0 \tag{4.44}$$

for positive $\frac{K_{C,i}}{C_i}$ as given in Chapter 2, if the algorithm is positive. The resulting dynamic behavior for the process networks and control algorithms is given as the gradient system

$$\frac{1}{C_1}\frac{dZ_1}{dt} = \frac{\partial P}{\partial Z_1} \tag{4.45}$$

$$\frac{1}{C_2}\frac{dZ_2}{dt} = \frac{\partial P}{\partial Z_2} \tag{4.46}$$

4.2 Decomposition of Process Networks

We now show, how two independent optimization problems are linked when the physical systems are connected as shown in Fig. 4.5. The optimization problem for each process network is given by

(3.29)

$$\min_{\mathbf{F}} \quad G = \int_0^{\mathbf{F}} \mathbf{W}^T d\mathbf{F} \tag{4.47}$$

$$s.t. \qquad \mathbf{AF} = \mathbf{0} \tag{4.48}$$

$$\mathbf{F} = \Lambda(\mathbf{W}) \tag{4.49}$$

We assume that the process network has two integrated connection structures given by the incident

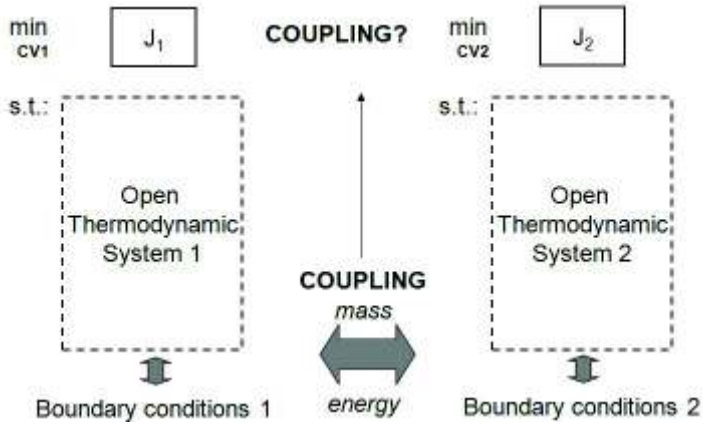

Figure 4.5: Two open thermodynamic system which can be separately optimized but once mass and energy between them is exchanged, communication between the two optimizers might be required.

matrices $\mathbf{A_1}$ and $\mathbf{A_2}$. The linking connection across the node i is given by

$$F_{1,i} + F_{2,i} = F_i^{total} \tag{4.50}$$

A graphical illustration of the process networks is given in Fig. 4.6. The optimization problem for

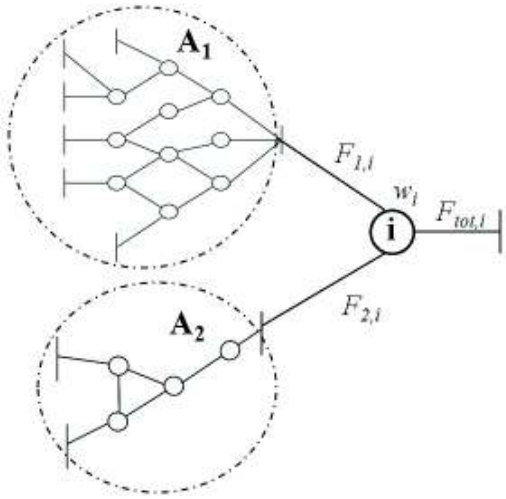

Figure 4.6: Two process networks connected through a single node.

the considered network then follows as

$$\min_{\mathbf{F_1},\mathbf{F_2}} \quad J = \int_0^{\mathbf{F_1}} \mathbf{W_1}^T d\mathbf{F_1} + \int_0^{\mathbf{F_2}} \mathbf{W_2}^T d\mathbf{F_2} \tag{4.51}$$

$$s.t. \qquad F_{1,i} + F_{2,i} = F_i^{total} \tag{4.52}$$

$$\mathbf{AF_1} = \mathbf{0} \tag{4.53}$$

$$\mathbf{AF_2} = \mathbf{0} \tag{4.54}$$

$$\mathbf{F_1} = \Lambda_1(\mathbf{W_1}) \tag{4.55}$$

$$\mathbf{F_2} = \Lambda_2(\mathbf{W_2}) \tag{4.56}$$

where the variables of the optimization problem for the process network 1 share one constraint with the process network 2. We formulate the relaxed problem as

$$\min_{\mathbf{F_1},\mathbf{F_2}} \quad J = \int_0^{\mathbf{F_1}} \mathbf{W_1}^T d\mathbf{F_1} + \int_0^{\mathbf{F_2}} \mathbf{W_2}^T d\mathbf{F_2} + w_i(F_i^{total} - F_{1,i} - F_{2,i}) \tag{4.57}$$

$$s.t. \qquad \mathbf{AF_1} = \mathbf{0} \tag{4.58}$$

$$\mathbf{AF_2} = \mathbf{0} \tag{4.59}$$

$$\mathbf{F_1} = \Lambda_1(\mathbf{W_1}) \tag{4.60}$$

$$\mathbf{F_2} = \Lambda_2(\mathbf{W_2}) \tag{4.61}$$

Theorem 10 in Chapter 3 shows that the potential at node i serves as the Lagrangean multiplier. We can therefore decompose the optimization problem into two separate problems using the method of Lagrangean decomposition

$$\min_{\mathbf{F_1}} \quad J_1 = \int_0^{\mathbf{F_1}} \mathbf{W_1}^T d\mathbf{F_1} + w_i(F_i^{total} - F_{1,i}) \tag{4.62}$$

$$s.t. \qquad \mathbf{AF_1} = \mathbf{0} \tag{4.63}$$

$$\mathbf{F_1} = \Lambda_1(\mathbf{W_1}) \tag{4.64}$$

and

$$\min_{\mathbf{F_2}} \quad J_2 = \int_0^{\mathbf{F_2}} \mathbf{W_2}^T d\mathbf{F_2} + w_i(F_i^{total} - F_{2,i}) \tag{4.65}$$

$$s.t. \qquad \mathbf{AF_2} = \mathbf{0} \tag{4.66}$$

$$\mathbf{F_2} = \Lambda_2(\mathbf{W_2}) \tag{4.67}$$

The Lagrangean multiplier w_i being the potential at node i follows directly from the dual optimization problem, see Chapter 3.

This result therefore shows that the optimality principles of a process network can be decomposed

into smaller units down to the single node or flow connection. The potentials as decomposition variables and Lagrangean multipliers play hereby an important role. The control system requires two types of control algorithms: One type of algorithm controls the flows directly as described in Section 4.1. The other type of algorithm has routing-type characteristics, receiving information from the flow controllers and determining capacities for the incoming and outgoing flows by adjusting the potential. The combination of a physical network and a control system with flow algorithms and routing algorithms has to be passive, i.e., each individual algorithm and the process network have to be passive to guarantee stability and optimality [10, 25].

In designing decentralized control schemes of large interconnected physical networks, some of the flows cannot be measured or controlled directly. Controlling or measuring all flows is in many cases not necessary, if the uncontrolled flows of the process network are "self-optimizing". In order to leave parts of the process network for self-optimization, the natural objective has to align with the desired engineering objective. For example, for the maximization of throughput, the natural objective minimizes dissipation and, hence, the maximization of flow throughput follows automatically. We derive the principle as follows from Tellegen's theorem. The dissipation from (3.9) in Chapter 3 is given as

$$\sigma_s = \sum_{i=1}^{n_f} F_i W_i \tag{4.68}$$

which is minimized for the steady state following from Corollary 3. Tellegen's theorem then gives

$$\sum_{i=1}^{n_f} F_i W_i = -(\sum_{i=1}^{n_T^{IN}} F_{Ti}^{IN} w_{Ti}^{IN} - \sum_{i=1}^{n_T^{OUT}} F_{Ti}^{OUT} w_{Ti}^{OUT}) \tag{4.69}$$

We use

$$\sum_{i=1}^{n_T^{IN}} F_{Ti}^{IN} = \sum_{i=1}^{n_T^{OUT}} F_{Ti}^{OUT} \tag{4.70}$$

from inventory conservation. Since all potentials at the terminals are fixed, we can express the termi-

nal contribution in Tellegen's theorem using the total flow

$$F_T^{total} = \sum_{i=1}^{n_T^{IN}} F_{Ti}^{IN} = \sum_{i=1}^{n_T^{OUT}} F_{Ti}^{OUT} \tag{4.71}$$

and assign an averaged potential difference across the process network

$$\sum_{i=1}^{n_T^{IN}} F_{Ti}^{IN} w_{Ti}^{IN} - \sum_{i=1}^{n_T^{OUT}} F_{Ti}^{OUT} w_{Ti}^{OUT} = F_T^{total} W^{avg} \tag{4.72}$$

It follows directly that minimizing the dissipation maximizes the flow through the network.

4.2.1 Illustrative Example: Network Model of a Petroleum Platform

We use a pipeline process network in the following example to demonstrate, how control can be decentralized and how the general optimization goal for operations are aligned with the self-optimizing property. A typical petroleum production system, as shown in Fig. 4.7, consists of (i) the reservoir, (ii) production wells, (iii) manifolds, (iv) flow lines to the surface, and (v) a first stage separator at some surface facility. Each well consists of three parts: The well tubing, the choke, and the well flow line. In Fig. 4.7 well flow may be routed to one out of two flow lines. Further, the production from a

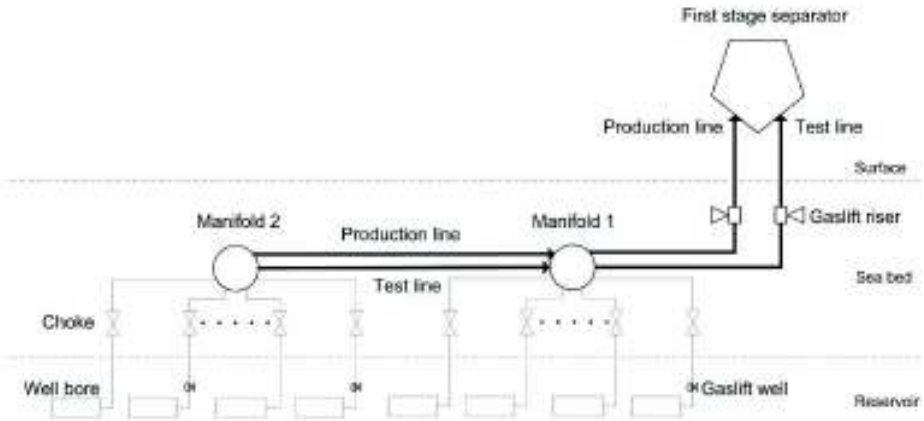

Figure 4.7: Model of topology for a typical oil and gas production system from [17].

well may be controlled by a production choke valve. An oil and gas field typically consists of a large number of productions systems.

The interconnection superstructure of the tree-like pipeline network is captured by the incident matrix **N**. The incident matrix contains binary decision variables for the switching between flow lines y_{ij}. For a given superstructure incident matrix **N**, we propose the following model based on Gunnerud et al. [17]:

Conservation laws:

$$\mathbf{N}\mathbf{q_o} = \mathbf{0} \tag{4.73}$$

$$\mathbf{N}\mathbf{q_g} = \mathbf{0} \tag{4.74}$$

$$\mathbf{N}\mathbf{q_w} = \mathbf{0} \tag{4.75}$$

Pressure relations:

$$\Delta\mathbf{p} = \mathbf{N}^T\mathbf{p}_{abs} \tag{4.76}$$

Reservoir to well inflow relations:

$$\Delta\mathbf{p}^{WELLBORE} = f(\mathbf{q_o}, \mathbf{q_g}, \mathbf{q_w}) \tag{4.77}$$

Pipeline pressure drops (momentum balances):

$$\Delta\mathbf{p}^{PIPELINE} = f(\mathbf{q_o}, \mathbf{q_g}, \mathbf{q_w}) \tag{4.78}$$

Choke pressure drops:

$$\mathbf{q_o} = f(\mathbf{d}^{\mathbf{CHOKE}}, \Delta\mathbf{p}^{\mathbf{CHOKE}}) \tag{4.79}$$

The conservation laws (4.73), (4.74), and (4.75) represent balances of the flow rates for oil $\mathbf{q_o}$, gas $\mathbf{q_g}$,

and water $\mathbf{q_w}$ for every node in the pipeline network. The pressure relations ensure that the pressure decreases according to the pressure drops from the reservoir pressure p^R to the separator pressure p^S along each path or sum up around each closed loop through the network.

Eqs. (4.73) - (4.75) and (4.76), representing the generalized Kirchhoff laws, for the pipeline network are linear and constitute the topological relations of the network. The pressure drop and inflow relations are commonly described through empirical or semi-empirical models. The momentum balance in the pipelines is typically given in form of discrete performance tables or measured data rather than analytical functions. Nonlinearities and dynamics of the system are introduced through (4.77)-(4.78). The parameters $\mathbf{d}^{\mathbf{CHOKE}}$ are continuous control parameters to adjust the flows through the wells. Further constraints during operation are imposed by the equipment. These constraints are mainly capacity limits for the oil, gas, and water flow in the pipelines and constraints imposed by the handling facilities at the surface. Boundary conditions for the model occur where the pipeline network is connected to the environment, i.e., the upstream boundary conditions apply as reservoir pressures for each well and downstream the separator pressure are given at the terminals. The free variables available for control and optimization are the choke openings as well as the discrete switches for the flow lines.

Dissipative Properties and Decentralized Control of Pipeline Flow

The total dissipation function from (3.9) for the pipeline network is given as the product of flows and pressure differences

$$E = \sum_{i=1}^{n_f} q_{total,i} \Delta p_i \tag{4.80}$$

In order to determine the potential function for the process network, the following optimization problem has to be considered

$$\min_{\mathbf{p}} \quad \int_0^{\Delta\mathbf{p}} \mathbf{q_o}^T d(\Delta\mathbf{p}) + \int_0^{\Delta\mathbf{p}} \mathbf{q_w}^T d(\Delta\mathbf{p}) + \int_0^{\Delta\mathbf{p}} \mathbf{q_g}^T d(\Delta\mathbf{p}) \tag{4.81}$$

$$s.t. \qquad \Delta\mathbf{p} = \mathbf{N^T p_{abs}} \tag{4.82}$$

$$\Delta\mathbf{p}^{WELLBORE} = f(\mathbf{q_o}, \mathbf{q_g}, \mathbf{q_w}) \tag{4.83}$$

$$\Delta\mathbf{p}^{PIPELINE} = f(\mathbf{q_o}, \mathbf{q_g}, \mathbf{q_w}) \tag{4.84}$$

$$\mathbf{q_o} = f(\mathbf{d}^{\mathbf{CHOKE}}, \Delta\mathbf{p}^{\mathbf{CHOKE}}) \tag{4.85}$$

$$\mathbf{p^R} = \text{const} \text{ ,and } p^{atm} = \text{const} \tag{4.86}$$

These expressions define the potential function $\Psi(\mathbf{p})$ using the methods derived in Chapter 3 implicitly. Due to the nonlinear and non-analytical functions for the pressure-flow relations (4.83), (4.84), and (4.85), an analytical expression cannot directly be derived from the optimization problem and has to be done numerically. We further do not expect $\Psi(\mathbf{p})$ to be a convex function of the pressures $\mathbf{p}$ due to the nonlinearities.

From a physical point of view, the pipeline network chooses the path of least resistance for oil, gas, and water flow corresponding to a (local) minimum of the potential function. Consequently, if all chokes are open, the friction in the pipeline network is minimized and the total mass flow through the network is maximized, i.e., the fluid production is simultaneously maximized. Due to capacity constraints, gas production has to be constrained such that the wells with the highest oil-to-gas ratio are operated at higher flow rates than the wells producing large amounts of gas and water. This introduces an aspect of selectivity into the process which would otherwise lead to a simple maximum throughput strategy. Hence, an efficient strategy selects the wells with the best oil-to-gas ratio while maximizing the total throughput by minimizing choking control action.

In order to coordinate production activities for these pipeline process networks, the pipeline and

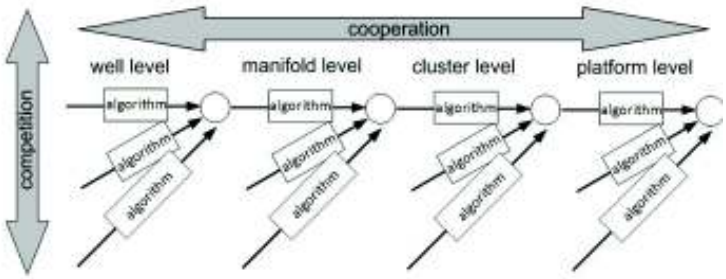

Figure 4.8: Decomposition of control tasks. Algorithms either directly control flows on lower levels or route flows at higher levels through assigning flow capacities.

reservoir flow has to be orchestrated through well choke settings to maximize the oil production and simultaneously meeting the gas capacity limit. Decomposition such as illustrated in Fig. 4.5 of the control objective for the entire platform can be achieved starting at the top of the pipeline hierarchy. Decomposing can be performed at every routing node into subproblems down to the well level, see Fig. 4.8. For example, Lagrangean decomposition in production optimization of a gas and oil platform in the North sea was carried out in [13]. Different control and optimization algorithms can be combined in the platform as long as input-output pairs of measurements and control can be shown as passive. Lower level controllers maximize oil production while satisfying capacity constraints imposed by the higher level routing algorithms.

A competitive system of algorithm for each hierarchical level is responsible for decision making, where the goal of each controller is to maximize the flow capacity that is assigned to it. The assignment of flow capacity is performed by a higher level decision makers where Lagrangean multipliers of the decomposed subproblems can be seen as shadow prices for which capacity is traded to lower level controllers. Consequently, the structure resembles a classical business environment in a market economy with entities competing over resources but exchanging information and cooperation with higher level optimizers similar to customers.

Chapter 5

Tellegen's Theorem and Global Optimization

"The field equivocally covered by the word communication
permits itself to be reduced massively by the limits
of what is called the context."

Jacques Derrida

In recent years, global nonlinear optimization has made advances in the context of developing algorithms for different classes of problems [29]. Although much progress has been made, the application of these algorithms still lacks efficiency for large scale problems. Especially, in the case of approaching dynamic systems, the discretization of partial differential equations classically found in process systems applications results in a large number of constraints. It is often argued that the nonconvexity can be surmounted by using a local method repeatedly, starting from a number of different initial decision vectors. Dependent on the complexity of the problem, even a large number of trials can miss the global solution and guarantees cannot be given. In this work, we develop a method assisting towards the solution of global optimization problems for dynamic flow networks. Typical systems

contain network structures of the type illustrated in this work, where nonlinear constitutive equations as well as nonconvex objective functions lead to nonlinear programs (NLPs).

Global optimization algorithms have been developed for a broad range of different nonlinear programs in recent times. In the given simultaneous approach, the system is fully discretized into a large scale NLP and solved using spatial branch and bound methods. In the area of deterministic global optimization methods, Esposito and Floudas [12] have recently solved nonlinear optimal control (dynamic optimization) problems. However, restrictions apply to the differentiability of the objective function and dynamic system and computational performance is strongly dependent on the type of nonlinearities and problem size. Furthermore, the size of the regarded problems and the type of nonlinearities that can be solved is fairly limited.

We investigate a method that enhances the efficiency of branch and bound algorithms for global optimization of these dynamic process networks. This work has as major objective to propose a methodology to generate formulations which lead to tighter convex relaxations of the regarded dynamic optimization problem. Ruiz and Grossmann [45] showed that the relaxation of nonconvex MINLPs can be strengthened systematically by using redundant constraints (i.e., generalized reduction constraints) obtained from alternative formulations using engineering knowledge and physical insight. Redundant formulations are classically disregarded in modeling and optimization of process systems and redundant constraints are commonly considered bad practice. However, the authors showed that using redundant formulations adds valuable information to the problem formulation, assists the solver, and can hence extend the size of problems that can be addressed towards larger scale applications. In this work, we build on the work of Ruiz and Grossmann [45] to extend it to dynamic systems by exploiting the alternative formulations that can be obtained by considering Tellegen's Theorem.

5.1 Global Optimization

Since the 1960s, several nonlinear programming algorithms have been proposed to solve optimization problems with nonlinear constraints [50]. However, most of them guarantee global optimality only, if the problem satisfies some convexity properties. General problems are nonconvex and the solutions obtained by the application of the traditional techniques are often local. Hence, in order to find the global optimum, specialized techniques are required which are usually based on convex relaxations of the nonconvexities in the regarded problems. In order to generate these relaxations, Tawarmalani and Sahinidis [50] proposed a methodology that consists of replacing the nonconvex terms by suitable convex envelopes.

The most common algorithm used to solve Mixed Integer Linear Programs (MILPs) and "nonconvex" NLPs are based on the branch and bound framework [21]. The fundamental difference between branch and bound algorithms for MILPs and the spatial branch and bound algorithms (sBBs) for nonconvex NLPs is that in the case of a nonconvex NLP, there is no single convex relaxation. Consequently, in the case of NLPs different formulations lead to different relaxations although the formulations are equivalent. It is an important topic to formulate an engineering optimization problem, where the convex relaxation is as tight as possible as compared to the original nonconvex problem. The computational efficiency of this methodology heavily rely on the quality of the relaxation. In general, the tighter the relaxation the more efficient the algorithm.

Better mathematical formulations for specific NLPs may be found on the basis of physical insight and intuition. However, it is clear that methods which result into a systematic approach of utilizing structural or physical information for wide classes of nonconvex NLPs would be highly desirable.

5.1.1 Global Optimization of Dynamic Systems

A particular optimization problem arises when its constraints are described through a set of differential equations. In general, these optimal control problems are nonconvex as shown by Papamichail

and Adjiman [40]. The authors proposed a methodology to find the global minimum by approaching the problem from above and below by generating converging sequences of upper and lower bounds. Local solutions, obtained using the sequential approach for the solution of the dynamic optimization problem, provide upper bounds. Lower bounds are produced from the solution of a convex relaxation of the original problem. Algebraic functions are relaxed using well-known convex underestimation techniques.

However, Esposito and Floudas [12] showed that global deterministic optimization of nonlinear optimal control problems requires conditions on the differentiability of the constraints and the objective function as well as on the index of the system. The authors showed that even for small size systems, a large number of local optima exist and make convergence of the used branch and bound algorithm extremely dependent on the relaxation.

It is apparent, that particularly for optimal control type problems with a large number of local optima, a formulation that can be approximated tightly through convex functions is desirable. In order to achieve this, we propose to exploit the network character of typical process systems in which flow is induced through potential gradients and hence certain topological properties apply.

5.1.2 Generalized Reduction Constraints

Typical optimization problems for these process systems contain a set of constraints for the network model and an objective function P specific to the particular application:

$$\min_{\mathbf{u}} \quad P(\mathbf{u_{ij}}, \mathbf{f}, \mathbf{w}) \tag{5.1}$$

$$s.t. \quad \sum \Delta w_{ij} = 0 \tag{5.2}$$

$$\frac{dZ_i}{dt} = \sum_{j=1}^{n_T} f_{Tj,i} + \sum_{j=1, j\neq i}^{n} f_{ij}(u) \tag{5.3}$$

$$f_{ij} = f(\Delta w_{ij}, u) \tag{5.4}$$

$$\mathbf{f_{Tj}} = \text{const and/or } \mathbf{w_{Tj}} = \text{const} \tag{5.5}$$

The objective function is classically some common optimization metric, i.e., a physical or economic cost function during the operation of the network. Our description of networks allows a clean separation of nonlinear and linear constraints, since the topological equations such as the conservation laws (2.25) and the uniqueness conditions (2.27) are by definition linear and the constitutive equations contain the nonlinearities. Dependent on the particular optimization problem, the objective function may be linear or nonlinear. In many network problems, the optimization problem is given as

$$\min_{\mathbf{u}} \quad P(\mathbf{u}) \tag{5.6}$$

$$s.t. \quad \mathbf{f}_1(\mathbf{u}) = \mathbf{0} \tag{5.7}$$

$$\mathbf{g}(\mathbf{u}) \leq \mathbf{0} \tag{5.8}$$

where the linear topological equations and the nonlinear constitutive equations are inseparable and combined in one general model of nonlinear differential equations $\mathbf{f}_1(\mathbf{u})$. The function $\mathbf{g}(\mathbf{u})$ typically represent capacity and other algebraic constraints which can be linear or nonlinear. In order to find a convex relaxation of the optimization problem, the set of equality constraints representing the model $\mathbf{f}_1(\mathbf{u})$ are approximated, for example in case of bilinear nonlinearities, by convex envelopes [33]. As a result, the convex relaxation of the constraints leads to a larger feasible region than for the original problem. In terms of computational expense, it is a significant advantage to limit the feasible region as close as possible to the original problem's feasible region. This is particularly important, if the solution of the relaxed problem lies outside of the original feasible region. As described in the work of Liberti [29] and Ruiz and Grossmann [45], reduction constraints are usually equations that function as cuts to the feasible region of the relaxed problem. If we have an optimization problem as given in (5.6) - (5.8), the generated additional redundant constraints $\mathbf{f}_2(\mathbf{u})$ are added to the initial set of

constraints resulting in

$$\min_{\mathbf{u}} \quad P(\mathbf{u}) \tag{5.9}$$

$$s.t. \quad \mathbf{f}_1(\mathbf{u}) = \mathbf{0} \tag{5.10}$$

$$\mathbf{f}_2(\mathbf{u}) = \mathbf{0} \tag{5.11}$$

$$\mathbf{g}(\mathbf{u}) \leq \mathbf{0} \tag{5.12}$$

Redundancy of model equations is generally not desired in engineering when building models. Nevertheless, redundant equations contain information and in the context of global optimization, additional redundant equations can be considered as important information for the algorithm or solver. The main challenge is to systematically find redundant constraints for particular systems or model realizations. As pointed out in [45], it is often necessary to use physical insight to find alternative model formulations. For systems with consistent network character, we can propose Tellegen's Theorem as alternative and redundant model equation. For the particular case of the network system, it follows

$$\min_{\mathbf{u}} \quad P(\mathbf{u}) \tag{5.13}$$

$$s.t. \quad \sum_{LOOP} \Delta w_{ij} = 0 \tag{5.14}$$

$$\frac{\Delta Z_i}{\Delta t} = \sum_{j=1}^{n_T} f_{Tj,i} + \sum_{j=1, j\neq i}^{n} f_{ij}(u) \tag{5.15}$$

$$f_{ij} = f(\Delta w_{ij,u_{ij}}) \tag{5.16}$$

$$\sum_{i=1}^{n_p} \frac{dZ_i(t_1)}{dt} w_i(t_2) = -\sum_{i=1}^{n_f} f_{ij}(t_1) \Delta w_i(t_2) \tag{5.17}$$

$$+\sum_{i=1}^{n_f} F_{Tj,i}(t_1) w_{Ti}(t_2) \tag{5.18}$$

$$f_{Tj,i} = \text{const and/or } w_{Tj,i} = \text{const} \tag{5.19}$$

where Tellegen's Theorem corresponds to $\mathbf{f}_2(\mathbf{u}) = \mathbf{0}$ in the general formulation. Tellegen's Theorem reduces the error of the convex approximation concerning the topological structure and energy bal-

ance which are lost in some parts of the relaxed space for the set of equations $\mathbf{f}_1(\mathbf{u}) = \mathbf{0}$. Tellegen's Theorem becomes particularly useful for dynamic optimization problems, since it holds combinations of the potentials of one state and the flows of the other state and vice versa as in (2.40).

The optimal model with the best relaxation is found for the case in which the set of equations are kept separate, i.e., the inventory balances and Kirchhoff's voltage law as linear equations are explicitly stated in the model and the constitutive equations which introduce nonlinearities and hence nonconvexities are separate. This results in much smaller number of open nodes of the branch and bound tree and the convergence of the gap between lower and upper bound is orders of magnitudes faster. For this particular type of formulation, Tellegen's theorem does not tighten the relaxation, since none of the linear Kirchhoff laws needs to be relaxed. In summary, a network formulation is superior to other formulations if the given model can be formulated keeping Kirchhoff equations and constitutive equations separate. However, in many dynamic model formulations, the different model components cannot be separated, so that a version of Tellegen's theorem adds strength to the relaxation and improves solvability.

5.2 Example: Dynamic Flow Network

An example was implemented to show the effect Tellegen's theorem has on strengthening the relaxations for the global optimization of a dynamic system. A schematic of the system can be seen in Fig. 2.4.

The system equations are given as (2.54) - (2.63). For numerical simplicity, the system parameters are chosen as $\rho g = 1$, $p_{atm} = 0$, $A_j = 1$, $\frac{\pi r_i^4}{8\eta} = 1$, $p_{T2} = p_{atm}$, $L_{1,2} = 4$, $t_F = 1.1$ and $L_{2,1} = L_{2,2} = 5$. The resistive constitutive equation according to (2.54) for the pipelines was set as a cubic function.

$$\dot{V}_i = \frac{1}{L_i}(0.096\Delta p_i^3 - 1.44\Delta p_i^2 + 5.8\Delta p_i) \tag{5.20}$$

Eq. (5.20) constitutes a locally active flow-pressure relationship. The function leads to a generally passive and hence stable behavior of the flow network, but exhibits several stationary points dependent on boundary and initial conditions. This equation is not based on physical principles; the coefficients are chosen so that the constitutive equation introduces nonconvexities into the optimization problem.

The system was implemented in GAMS as the following ordinary differential equations (ODEs) derived from (2.54) to (2.63):

$$\frac{dp_j}{dt} = \dot{V}_i^{in} - \dot{V}_i^{out} \tag{5.21}$$

We assume positive flow across the network with terminal T_1 being the location of highest pressure as an inventory source and terminal T_2 being the lowest pressure point which results in the inequality constraint

$$p_{T1} \geq p_{1,2} \geq p_{T2} \tag{5.22}$$

as part of the model.

Tellegen's theorem for this system can be can be derived from (2.41) as

$$\sum_{i \in \text{tanks}} p_i(t_2) \frac{dV_i(t_1)}{dt} = \sum_{i \in \text{tanks}} p_i(t_2)\dot{V}_i^{in}(t_1) - \sum_{i \in \text{tanks}} p_i(t_2)\dot{V}_i^{out}(t_1) + \sum_{i \in \text{terminals}} p_i(t_2)\dot{V}_i^{in}(t_1) - \sum_{i \in \text{terminals}} p_i(t_2)\dot{V}_i^{out}(t_1) \tag{5.23}$$

where the summation terms have been expanded using the problem topology, and the sign changed accordingly. Eq. (5.23) was implemented using only pressure (state) variables, by substituting flows and volumes in Tellegen's theorem. The fully implicit Euler method was chosen as the discretization

scheme for simplicity and numerical stability. For $dp/dt = f(p(t))$,

$$\frac{p_j(k+1) - p_j(k)}{T} = \dot{V}_i^{in}(k+1) - \dot{V}_i^{out}(k+1) \tag{5.24}$$

where k represents discrete time.

The power dissipation at final time t_F was chosen as the minimized objective:

$$P(L_{11}, p_{T1}) = \sum_{\text{pipes}} \dot{V}(t_F)\Delta p(t_f) \tag{5.25}$$

The optimization problem has multiple local minima at $P^{min,1} = 15.27$ for $p_{T1}^{min,1} = 9.911$ and $L_{1,1}^{min,1} = 10$, and $P^{min,2} = 16.69$ for $p_{T1}^{min,2} = 7$ and $L_{1,1}^{min,2} = 7$ (at the boundaries), as shown in Fig. 5.1. The global optimum is at $P^{globalmin} = 14.453$, with $p_{T1}^{globalmin} = 7$ and $L_{1,1}^{globalmin} = 1$. The power dissipation is lower for smaller values of pressure in Terminal T_1.

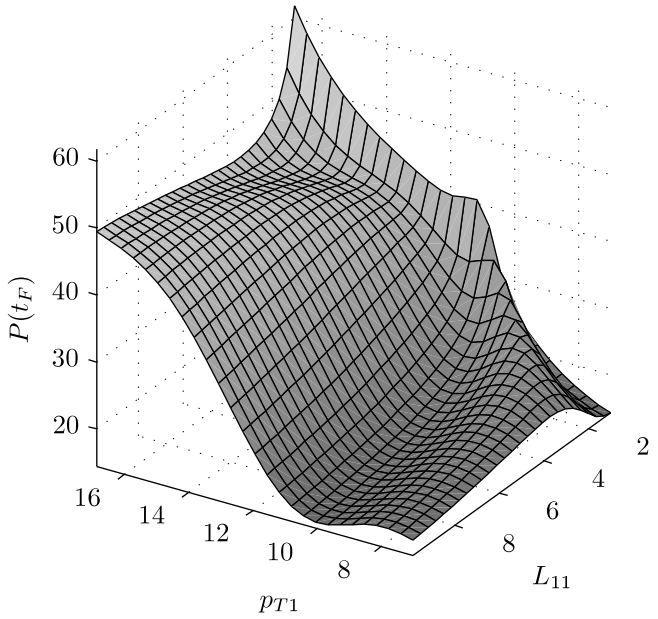

Figure 5.1: Surface plot of the objective function.

The ODE system was solved with the global optimizer BARON 8.5.1 [51], with $7 \leq p_{T1} \leq 17$

and $1 \leq L_{1,1} \leq 10$ as decision variables, and initial conditions $p_1(0) = p_2(0) = 4$. The reference implementation consisted of Eq. (5.20) - (5.22), i.e., no redundant equations. The system was also implemented with Tellegen's theorem as a redundant constraint, with $t_1 = t_2$, which corresponds to a power balance. Eq. (5.23) was included as a "relaxation-only constraint" not used for feasibility testing or local searching through BARON's `eqclass` option being active.

The problem was solved on an Intel T2600 (two 2.16 GHz CPUs) with 1 GB of RAM. For both model implementations, BARON's probing parameter was set to `PDo` $= 10$ as the number of variables to probe on. All other BARON options were left to their defaults; MINOS and CPLEX were used as NLP and LP solvers, respectively. Both implementations converged to the global optimum $P^{globalmin}$, which can be verified through Fig. 5.1 as the global optimum.

Fig. 5.2 compares how the lower bound converges to the upper bound for both implementations, plotted against iteration number. For any iteration during the optimization process, the lower bound given calculated with Tellegen's theorem was higher than without, illustrating the strengthening of the feasible region's relaxation through Tellegen's theorem as a redundant constraint. Fig. 5.3 compares

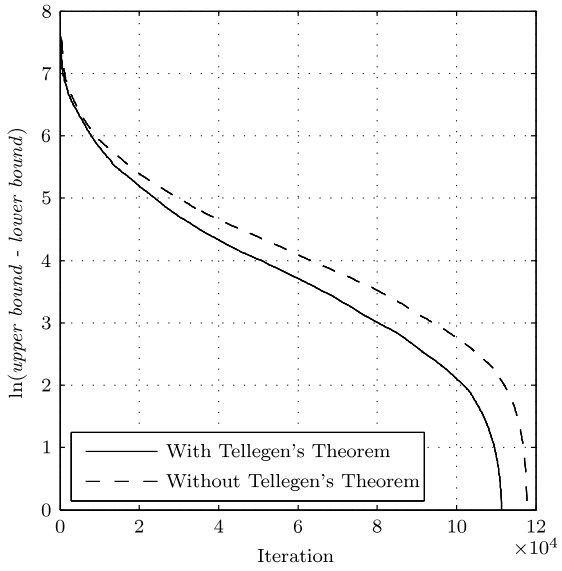

Figure 5.2: The difference between upper and lower bounds with and without Tellegen's theorem as a redundant constraint, plotted on a logarithmic scale.

the number of open nodes in the branching tree for both implementations, plotted against the iteration number. When Tellegen's theorem was used as a redundant constraint, the number of open nodes was smaller for any iteration throughout the optimization run. This indicates that BARON can discard nodes more effectively as Tellegen's theorem helps tightening the relaxation. The number of iterations

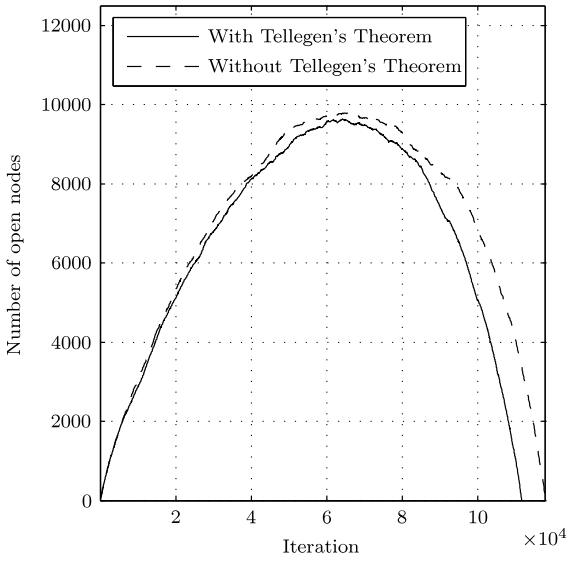

Figure 5.3: Comparison of the number of open nodes with and without Tellegen's theorem as a redundant constraint.

when using Tellegen's theorem in the formulation was smaller ($n_{iter}^{Tellegen} = 111,690$) as compared to without Tellegen's theorem ($n_{iter} = 117,951$).

In conclusion, we note an improvement in the gap between lower bound and upper bound of the problem as well as the number of branching nodes during the optimization process. This shows that if the system of difference equations given by (5.21) is relaxed through convex approximations, the feasible region of the resulting relaxed NLP contains regions that violate Tellegen's theorem. The addition of Tellegen's theorem to the optimization problem thus functions as cuts to the feasible region reducing the size of the hypervolume of the relaxation. In this particular case, Tellegen's theorem was applied as a power balance. Although the addition of Tellegen's theorem increases the problem size, we show that the principle holds potential to impact the tightness of the final relaxation.

Chapter 6

Two-phase Flow in Porous Media

”Our ignorance is not so vast

as our failure to use what we know.”

Marion King Hubbert

6.1 Subsurface Flow Modeling

Reservoir flow behavior is governed by the conservation of mass, momentum, and energy. The numerical solution of these equations is extremely difficult in the complete form [3] and is typically executed using commercial software like ECLIPSE[1]. A range of assumptions and simplifications as well as a discretization in space and time is commonly performed. A common approach in reservoir engineering is the assumption of an isothermal reservoir, i.e., the energy balance modeling the dynamics of the temperature in the reservoir is neglected. In addition, we assume that reservoir flow is

[1]ECLIPSE is an oil and gas reservoir simulator originally developed by ECL (Exploration Consultants Limited) and currently owned, developed, marketed and maintained by SIS (formerly known as GeoQuest), a division of Schlumberger. The name ECLIPSE originally was an acronym for ”ECLs Implicit Program for Simulation Engineering” [54].

slow and the accumulation term for the momentum balance can be disregarded. Further simplifications lead to Darcy's law as a constitutive equation that relates potential gradients to flow.

We consider isothermal flow of weakly compressible two phase liquid (oil-water) through a weakly compressible porous medium. The control volume $dV = dxdydz$ for the mass balance is assumed to be cubic or cuboid. We write the mass balance per unit time for the control volume dV as

$$\frac{\partial M^w}{\partial t} = \dot{M}^w_x|_x - \dot{M}^w_x|_{x+dx} + \dot{M}^w_y - \dot{M}^w_y|_{y+dy} + \Psi^w \tag{6.1}$$

$$\frac{\partial M^o}{\partial t} = \dot{M}^o_x|_x - \dot{M}^o_x|_{x+dx} + \dot{M}^o_y - \dot{M}^o_y|_{y+dy} + \Psi^o \tag{6.2}$$

Introducing the density $\rho^{o,w}$ where the superscript o stands for oil and w for water and the porosity $\phi = \frac{V^{liquid}}{V^{total}}$

$$\frac{(\partial \phi \rho^w S^w)}{\partial t} = -\frac{(\rho^w v^w_x)}{\partial x} - \frac{(\rho^w v^w_y)}{\partial y} + \rho^w q^w \tag{6.3}$$

$$\frac{(\partial \phi \rho^o S^o)}{\partial t} = -\frac{(\rho^o v^o_x)}{\partial x} - \frac{(\rho^o v^o_y)}{\partial y} + \rho^o q^o \tag{6.4}$$

The mass balance equations (6.1) and (6.2) balance the in- and outflux of mass through the boundaries in x-, y-direction for the control volume dV. We introduce a source/sink term q as boundaries to model wells as flow rate per unit volume and the so called Darcy velocity $v^{o,w}$. The water/oil saturation $S^{o,w}$ is defined as the proportion of pore space occupied by the respective phase.

The actual driving force of viscous flow through porous media is governed by potential gradients in the force field. Darcy's law is derived from the Navier-Stokes equation given by

$$\vec{v}^w = -\frac{k^w(S^w)}{\mu^w}\vec{k}\nabla p^w \tag{6.5}$$

$$\vec{v}^o = -\frac{k^o(S^o)}{\mu^o}\vec{k}\nabla p^o \tag{6.6}$$

where k is the rock permeability and μ is the fluid viscosity. The parameters $k^{o,w}(S^{o,w})$ are the relative permeabilities which represent the additional resistance to flow of a phase caused by the presence of the other phase. Darcy's law acts as a constitutive equation relating flow and potential gradients. Through Darcy's law, we introduced a set of intensive variables, here the pressure, which describe potentials and potential gradients at a certain location in the reservoir.

In order to complete the set of equations, it is necessary to introduce another type of constitutive relations which relate intensive variables like the pressure p to extensive variables such as the mass M or volume V at a defined location in the reservoir. Commonly, these capacitive constitutive equations are thermodynamic equations of state (EOS). These equations are of the form $p = f(V,T)$ or $p = f(\rho,T)$ and relate the variables pressure, temperature and volume (or density). Since we assume an isothermal reservoir, the EOS is a function of the form $p = f(\rho)$ or $p = f(V)$. There is a multitude of EOS available for different fluids dependent on its compressibility, composition etc.

In the case of a reservoir fluid, we formulate the equation of state for a liquid in its differential form as

$$c_l(p) = \frac{1}{\rho}\frac{\partial \rho}{\partial p}|_{T_0} \tag{6.7}$$

where $c_l(p)$ is the isothermal liquid compressibility and T_0 is a constant reference temperature, for which the reservoir temperature T_R is the most useful choice. We introduce an equation of state for the rock compressibility

$$c_r(p) = \frac{1}{\phi}\frac{\partial \phi}{\partial p}|_{T_0} \tag{6.8}$$

The compressibilities for fluid c_l and rock c_r can be summarized as the total compressibility c_t.

The coupling of the phases leads to two algebraic relationships, one between the extensive variables (volumes, saturations) and one between the intensive variables (pressure). The saturation S^w is defined as the fraction of water volume per total liquid volume in the free space of the pores

$S^w = \frac{V^w}{V^{liquid}}$. The oil saturation S^o is defined analogously as $S^o = \frac{V^o}{V^{liquid}}$

$$S^w + S^o = 1 \tag{6.9}$$

$$p^w - p^o = p^c(S^w) \tag{6.10}$$

The partial differential equations describe a vector field for the pressure and saturations as a function of time and space.

6.1.1 Single-phase Flow Network Model

Discretization in space using a finite difference or finite volume method allows us to introduce matrix algebra to describe the relevant equations and simplifies the mathematical structures. We first introduce the principle of spatial discretization into gridblocks for one liquid phase and subsequently extend the concept to water-oil two phase flow.

We discretize the 3-dimensional domain into cubic or cuboid grid blocks in the x, y, and z coordinates with the finite volume method. Since we regard only horizontal 2D flow, we will disregard the z coordinate along with gravitational forces. We define the subscripts i and j for the grid block numbering in x and y direction. The resulting mass balance for a grid block follows directly from (6.1) and (6.2)

$$\frac{dM_{ij}}{dt} = \dot{M}_{i-1j,ij} - \dot{M}_{ij,i+1j} + \dot{M}_{ij-1,ij} - \dot{M}_{ij,ij+1} + Q_{ij} \tag{6.11}$$

where the mass flows $\dot{M}$ enter and leave through the grid block boundaries in each spatial directions indicated in Fig. 6.1. The term Q accounts for possible sinks or sources such as wells that inject or produce fluids located in the grid block. The discretization converts the mathematical formulation from a distributed into a lumped parameter representation of the reservoir. Consequently, the

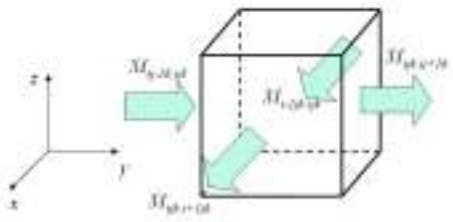

Figure 6.1: Gridblock ij with incoming and outgoing mass flows through the boundary surfaces to and from other grid blocks.

formulation of Darcy's law (6.5) and (6.6) can be simplified to

$$v_{ij,i+1j} = -\frac{k_{ij,i+1j}}{\mu\Delta x}\Delta p_{ij,i+1j} \quad \text{x-coord.} \tag{6.12}$$

$$v_{ij,ij+1} = -\frac{k_{ij,ij+1}}{\mu\Delta y}\Delta p_{ij,ij+1} \quad \text{y-coord.} \tag{6.13}$$

Due to the smoothness of the pressure field $\mathbf{p}$ in the spatial coordinates, the continuous formulation naturally obeys Kirchhoff's voltage law. Kirchhoff's voltage law is equivalent to the statement that a single-valued pressure potential can be assigned to each point in the reservoir (in the same way that any conservative vector field can be represented as the gradient of a scalar potential). In the discretized form, Kirchhoff's voltage law is established through the definition of the pressure differences

$$\Delta p_{ij,i+1j} = p_{ij} - p_{i+1j} \tag{6.14}$$

where the pressures correspond to the individual pressures of two connected grid blocks. The summation of all pressure differences along any closed loop of gridblocks in the reservoir is zero according to Kirchhoff's voltage law.

Conservation Property

The topology of a thermodynamic process, here a reservoir during injection, plays a crucial role in defining its properties. For the dynamic behavior, the "geology", i.e., the connective structure of the reservoir, is equally important as the functions between the state variables which we call the constitutive equations. In order to capture the connection structure of the gridblocks, we introduce a matrix that relates grid blocks and flows across grid block boundaries, as in Definition 2 in Chapter 2. The connections between gridblocks through flows can be uniquely defined using the connection matrix $\mathbf{A}$. Let Σ be a convex sub-set of $\mathbb{R}^n_+$ and let $\mathbf{M} = (M_1, ..., M_n)$ represent an arbitrary point. A vector $\mathbf{M}$ can be regarded as the mass inventory of n different gridblocks of the reservoir. We regard the gridblock as the smallest elementary reservoir. The vectors $\dot{\mathbf{M}}_i$ can be thought of as material flows across gridblocks and through wells. The state of the reservoir evolves according to the conservation laws

$$\frac{d\mathbf{M}}{dt} = \sum_{i=1}^{m} \dot{\mathbf{M}}_i(\mathbf{M}, \mathbf{u}, \mathbf{d}),\ \mathbf{M}(0) = \mathbf{M}_0 \tag{6.15}$$

$$y = h(\mathbf{M}) \tag{6.16}$$

The vector $\mathbf{M_0}$ is the initial condition, the vectors $\dot{\mathbf{M}}_i$, $i = 1, ..., n$ denote flows. We define a network of reservoir gridblocks in which each gridblock is regarded as an elementary process. Based on the connection matrix definitions, we write a general matrix equation for the conservation property:

$$\mathbf{AF} = \mathbf{0} \tag{6.17}$$

for the node-to-branch incident matrix $\mathbf{A}$, where $\mathbf{F^T} = [\frac{d\mathbf{M}^T}{dt}, \mathbf{Q}^T, \dot{\mathbf{M}}_\mathbf{y}, \dot{\mathbf{M}}_\mathbf{x}]$. The vectors of flows $\dot{M}_{xy}$ represent connections between two gridblocks in xyz-direction, i.e. $\dot{M}_{ij,i+1j}$ connects gridblock (ij) to gridblock $(i+1\,j)$ in x-direction and is a scalar element of vector $\dot{M}_x$, $\mathbf{Q}$ denotes sources or sinks which are effectively the injection and production wells. Eq. (6.17) corresponds to Kirchhoff's

current law (KCL) of electrical circuit theory in a generalized form with the inventory M_{ij} for each gridblock ij.

Reservoir Entropy

The second important network property is the uniqueness condition (Kirchhoff voltage law) for the complete reservoir. A potential follows directly through Euler's theorem from the entropy as

$$\mathbb{S}(\mathbf{M_i}) = \mathbf{M_i}^T \frac{\mathbf{p_i}}{\rho_\mathbf{i}} \tag{6.18}$$

For the definition of the potentials we derive the entropy for a weakly compressible fluid or solid. The entropy contributions for water, oil, and porous rock are given as

$$\mathbb{S}^{o,w,r} = Nk \left[\ln \left(\frac{V^{\alpha U^{c_v}}}{N^{\alpha + c_v}} \right) - \beta \frac{V}{N} \right] \tag{6.19}$$

where k is Boltzmann's constant and c_v is the specific heat capacity at constant volume, α is the thermal expansion, and β is the compressibility. A full derivation of the reservoir's entropy is given in App. E.2. The density as a function of pressure and compressibilities is derived from (6.19) and gives

$$\rho^{o,w,r} = \rho_0^{o,w,r} + c^{o,w,r}(p - p_0) \tag{6.20}$$

with $c = 1/\alpha T$ and

$$\rho_0^{o,w,r} = \frac{\beta}{\alpha} + \frac{1}{\alpha}\left(\frac{p_0}{T}\right)$$

Thus, (6.20) defines a weakly compressible fluid. For the reservoir, we have

$$\mathbb{S} = S^w \phi \mathbb{S}^w + S^o \phi \mathbb{S}^o + (1-\phi)\mathbb{S}^r - S^w \phi \ln(S^w \phi) - S^o \phi \ln(S^o \phi) + (1-\phi)\ln(1-\phi) \tag{6.21}$$

where $p_w = p_o = p_r$ and $T_w = T_o = T_r$.

Potentials and Uniqueness Property

Due to the definition of mass $\mathbf{M}$ as inventory, we will define potentials given as $w_i = \frac{p_i}{\rho_i}$ respectively. The uniqueness condition of the problem follows as

$$\mathbf{W}^T = [\rho^{-\mathbf{1}}\mathbf{p}, \rho_{\mathbf{Q}}^{-\mathbf{1}}\mathbf{p}_{\mathbf{Q}}, \bar{\rho}_x^{-1}\Delta\mathbf{p}_{\mathbf{x}}, \bar{\rho}_y^{-1}\Delta\mathbf{p}_{\mathbf{y}}]$$

In a thermodynamic sense, this definition plays an important role in terms of consistency with the definition of the mass being the conserved extensive variable. In our framework, stability and optimality results follow directly from the assumption that the state variables are defined as invariants. The uniqueness conditions follows as

$$\mathbf{W} = \mathbf{A}^T\mathbf{w} \tag{6.22}$$

The potentials $\mathbf{w}$ and potential differences $\mathbf{W}$ can be regarded as normalized pressures.

Single-phase Reservoir Differential Equation System

In case the reservoir fluid is weakly compressible and the density can be regarded as constant, we define the pressure p as potential and the volume V as inventory. In the general case, a definition consistent with the network assumptions can only be performed using the masses as inventories. The incident matrix $\mathbf{A}$ and the vector $\mathbf{F}^T = [\frac{d\mathbf{M}^T}{dt}, \mathbf{Q}^T, \dot{\mathbf{M}}_{\mathbf{y}}, \dot{\mathbf{M}}_{\mathbf{x}}]$ can be decomposed according to the following scheme

$$\mathbf{A} = \begin{bmatrix} \mathbf{I}^{\mathbf{n_p}\times\mathbf{n_p}} & \mathbf{L} & \mathbf{A}_{\mathbf{x}} & \mathbf{A}_{\mathbf{y}} \end{bmatrix}$$

This allows reformulation of (6.17):

$$\frac{d\mathbf{M}}{dt} = -\mathbf{A}_{\mathbf{x}}\dot{\mathbf{M}}_{\mathbf{x}} - \mathbf{A}_{\mathbf{y}}\dot{\mathbf{M}}_{\mathbf{y}} - \mathbf{A}_{\mathbf{z}}\dot{\mathbf{M}}_{\mathbf{z}} - \mathbf{L}\mathbf{Q} \tag{6.23}$$

Using Darcy's law, the constitutive equations, and several assumptions for the density explicitly given in App. E.3, we derive the resulting nonlinear ordinary differential equation to

$$\mathbf{V}(\mathbf{p})\frac{d\mathbf{p}}{dt} = \mathbf{T}(\mathbf{p})\mathbf{p} + \mathbf{Q}^* \tag{6.24}$$

The reservoir model described in this section is a general description of the reservoir dynamics for single phase flow in two dimensions. App. E.3 shows the formalism for a basic reservoir system.

Tellegen's Theorem for Single Phase Flow

In this section, we develop Tellegen's Theorem for the network based reservoir description.

Theorem 25. *For a reservoir with the topology described by the connection matrix* $\mathbf{A}$*,*

$$\sum_{i=1}^{n_f} F_i W_i = \mathbf{W}^T\mathbf{F} = 0 \tag{6.25}$$

where $\mathbf{F}^T = [\frac{d\mathbf{M}}{dt}, \mathbf{Q}, \dot{\mathbf{M}}_\mathbf{x}, \dot{\mathbf{M}}_\mathbf{y}]$ *and* $\mathbf{W}^T = [\rho^{-\mathbf{1}}\mathbf{p}^T, \rho_\mathbf{Q}^{-\mathbf{1}}{\mathbf{p}_\mathbf{Q}}^T, \bar{\rho}_x^{-1}\Delta\mathbf{p}_\mathbf{x}, \bar{\rho}_y^{-1}\Delta\mathbf{p}_\mathbf{y}]$

Proof. See 2.2.4. □

In this context Tellegen's theorem represents a power balance or a "balance of entropy dissipation" in the thermodynamic sense. The expanded version of Tellegen's theorem is given as

$$\mathbf{p}^T\rho^{-1}\frac{d\mathbf{M}}{dt} = -\Delta\mathbf{p}^T\bar{\rho}^{-1}\dot{\mathbf{M}} - {\mathbf{p}_\mathbf{Q}}^T\rho_Q^{-1}\mathbf{Q} \tag{6.26}$$

The term of the left hand side is a accumulation term $\mathbf{p}^T\rho^{-1}\frac{d\mathbf{M}}{dt}$ for the storage of potential energy in the grid cells. On the right hand side, there are three terms for in- and outflux of power: Resistive terms for the energy dissipation through percolation of the fluid $\Delta\mathbf{p}^T\bar{\rho}^{-1}\dot{\mathbf{M}}$, and power input/output through the wells ${\mathbf{p}_\mathbf{Q}}^T\rho_Q^{-1}\mathbf{Q}$.

6.1.2 Stability of Reservoir Dynamics

Prigogine [44] and Glansdorff [15] showed that for a wide range of dynamical systems, the quantity

$$dP_x = \sum F_i \dot{W}_i \leq 0 \tag{6.27}$$

holds during the natural evolution of a a non-equilibrium system toward a steady state. The equality only holds for the steady state. A typical dynamical system of this kind consists of flows F_i and gradients W_i and we observe that the dissipation of energy along a dynamic trajectory and along with it the change of gradients $\dot{W}_i$ decreases until it vanishes and reaches a local minimum, i.e. steady state of the system. Petroleum reservoirs can be seen as systems which typically fit in the framework of flows and gradients and in the context of oil production exhibit behavior of classical non-equilibrium systems. We therefore prove the following theorem for a reservoir with fixed potentials at the boundaries, i.e., pressures at the wells:

Theorem 26. *Given a single phase flow reservoir obeying constant pressures* $\mathbf{p}_Q$ *at the wells, the following inequality holds and the reservoir shows convergence to a unique solution in case of monotonous capacitive constitutive equations (equation of state)*

$$dP_w = \frac{\partial}{\partial t}(\Delta \mathbf{p}^T \bar{\rho}^{-1})\dot{\mathbf{M}} \leq \mathbf{0} \tag{6.28}$$

if the product of pressure and fluid compressibilities is

$$\mathbf{p}^T \mathbf{c_l} \leq 1 \tag{6.29}$$

Proof. See App. E.6 □

The change of dissipative quantities is therefore always negative for weak compressiblity of the fluids and decreases until it reaches the steady-state which minimizes the dissipation. The previously

introduced cocontent can be used to derive a Lyapunov function for the reservoir.

Theorem 27. *For a single phase reservoir, a Lyapunov candidate function is derived from the reservoir's cocontent*

$$G_R^* = \int^{\mathbf{W_R}} \mathbf{F_R}^T d\mathbf{W_R} = \int^{\bar{\rho}^{-1}\Delta\mathbf{p}} \dot{\mathbf{M}}^{\mathbf{T}} d(\bar{\rho}^{-1}\Delta\mathbf{p})$$

and the reservoir is globally asymptotically stable in the Lyapunov sense for monotonous constitutive equations (equation of state and Darcy's law) and constant pressures at the wells.

Proof. See App. E.7 □

The theorem confirms that a petroleum reservoir shows asymptotically stable behavior, if the fluids characteristics stay below a certain compressibility limit. We show in the following sections, that the resulting Lyapunov function constitutes the basis for a gradient system description of the reservoir.

6.1.3 Two-phase Flow Network Model

A two-dimensional geometry of the reservoir domain with wells being considered as point sources and sinks is considered. For a two-phase oil-water reservoir model, we have the following set of equations:

Mass balances:

$$\frac{d\mathbf{M}^w}{dt} = -\mathbf{A_x}\mathbf{M_x^w} - \mathbf{A_y}\mathbf{M_y^w} + \mathbf{L}\mathbf{Q^w} \tag{6.30}$$

$$\frac{d\mathbf{M}^o}{dt} = -\mathbf{A_x}\mathbf{M_x^o} - \mathbf{A_y}\mathbf{M_y^o} + \mathbf{L}\mathbf{Q^o} \tag{6.31}$$

Kirchhoff voltage law:

$$\Delta \mathbf{p}_{\mathbf{x}} = \mathbf{A}_{\mathbf{x}}{}^{T}\mathbf{p} \tag{6.32}$$

$$\Delta \mathbf{p}_{\mathbf{y}} = \mathbf{A}_{\mathbf{y}}{}^{T}\mathbf{p} \tag{6.33}$$

A common approximation for the life-cycle scale is to assume the capillary pressure $p^c = 0$ so that $\mathbf{p}^w = \mathbf{p}^o$. The resistive constitutive equations relating mass flow $\dot{\mathbf{M}}$ and pressure difference $\Delta\mathbf{p}$ are derived based on Darcy's law

$$v_{\mathbf{x},\mathbf{y}} = -\frac{1}{\mu \Delta x, y}\bar{\mathbf{k}}_{\mathbf{x},\mathbf{y}}\Delta \mathbf{p}_{\mathbf{x},\mathbf{y}} \tag{6.34}$$

The definition for flow velocity $v_{\mathbf{x},\mathbf{y}} = \frac{\dot{\mathbf{V}}_{\mathbf{x},\mathbf{y}}}{\Delta x h}$ and density $\dot{\mathbf{M}}_{\mathbf{x},\mathbf{y}} = \bar{\rho}_{\mathbf{x},\mathbf{y}}\dot{\mathbf{V}}_{\mathbf{x},\mathbf{y}}$ in combination with (6.34) gives the resistive constitutive equations.

Resistive constitutive equations:

$$\dot{\mathbf{M}}_{\mathbf{x}} = \frac{\Delta y h}{\Delta x \mu}\rho_{\mathbf{x}}\bar{\mathbf{k}}_{\mathbf{x}}\Delta \mathbf{p}_{\mathbf{x}} \tag{6.35}$$

$$\dot{\mathbf{M}}_{\mathbf{y}} = \frac{\Delta x h}{\Delta y \mu}\rho_{\mathbf{y}}\bar{\mathbf{k}}_{\mathbf{y}}\Delta \mathbf{p}_{\mathbf{y}} \tag{6.36}$$

For the capacitive constitutive equations, we relate mass $\mathbf{M}$ and pressure $\mathbf{p}$ through the definition of the density $\mathbf{M} = \rho\phi\mathbf{V}$, and an equation of state for the density $\rho = \rho(p)$ and porosity $\phi = \phi(p)$, see App. E.4.

$$\mathbf{M} = \rho(p)\phi(p)\mathbf{V} \tag{6.37}$$

The relation between mass, pressure, and volume in differential form can be derived as the capacitive constitutive equations, here as an extended equation of state, see App. E.4.

Capacitive constitutive equation:

$$\frac{d\mathbf{M}^w}{dt} = \rho\phi\left(\frac{d\mathbf{V}^w}{dt} + \mathbf{V}^w(\mathbf{c}^r + \mathbf{c}^w)\frac{d\mathbf{p}}{dt}\right) \tag{6.38}$$

$$\frac{d\mathbf{M}^o}{dt} = \rho\phi\left(\frac{d\mathbf{V}^o}{dt} + \mathbf{V}^o(\mathbf{c}^r + \mathbf{c}^o)\frac{d\mathbf{p}}{dt}\right) \tag{6.39}$$

Subsurface Flow System of Differential Algebraic Equations

The resulting differential algebraic equation (DAE) system is given as

$$V\phi\frac{d\mathbf{S}^w}{dt} + V\mathbf{S}^{wT}\phi(\mathbf{c}^r + \mathbf{c}^w)\frac{d\mathbf{p}}{dt} = -\mathbf{T}^w\mathbf{p} + \mathbf{Q}^w \tag{6.40}$$

$$V\phi\frac{d\mathbf{S}^o}{dt} + V\mathbf{S}^{oT}\phi(\mathbf{c}^r + \mathbf{c}^o)\frac{d\mathbf{p}}{dt} = -\mathbf{T}^o\mathbf{p} + \mathbf{Q}^o \tag{6.41}$$

$$\mathbf{T}^{o,w} = \mathbf{T}_{\mathbf{x}}^{\mathbf{o,w}} + \mathbf{T}_{\mathbf{y}}^{\mathbf{o,w}} \tag{6.42}$$

$$\mathbf{T}_{\mathbf{x}}^{\mathbf{o,w}} = \frac{\Delta y h}{\Delta x \mu^{o,w}}\mathbf{A_x}\mathbf{k}_{\mathbf{x}}^{\mathbf{o,w}}\mathbf{A_x}^T \tag{6.43}$$

$$\mathbf{T}_{\mathbf{y}}^{\mathbf{o,w}} = \frac{\Delta x h}{\Delta y \mu^{o,w}}\mathbf{A_y}\mathbf{k}_{\mathbf{y}}^{\mathbf{o,w}}\mathbf{A_y}^T \tag{6.44}$$

$$\mathbf{Q}^{o,w} = \mathbf{L}\mathbf{k}_{\mathbf{well}}^{\mathbf{o,w}}\mathbf{q}^{total} \tag{6.45}$$

$$\mathbf{q}^{total} = \mathbf{J}(\mathbf{p}^{gb} - \mathbf{p}^{well}) \tag{6.46}$$

$$\mathbf{k}_{\mathbf{x,y}}^{\mathbf{o,w}} = \mathbf{k_{x,y}}\mathbf{k_{ro,w}}(\mathbf{S^{o,w}}) \tag{6.47}$$

Equations (6.40) and (6.41) follow from the mass balances for water (6.30) and oil (6.31) in combination with Darcy's law (6.35) and (6.36) and the differential equations for compressibility of rock, water, and liquid (6.38) and (6.39). The matrices $\mathbf{T}_x(\mathbf{S})$ and $\mathbf{T}_y(\mathbf{S})$ represent the topology of the flow between gridblocks and are dependent on the water and oil saturation. The subscripts x and y represent the flows in the respective x and y directions in the reservoir. The vectors $\mathbf{Q}^w$ and $\mathbf{Q}^o$ represent the flow of oil and water through the wells and are also dependent on the saturation of oil and water in the near well region. The relative permeabilities are calculated using the Corey model given in App.

E.8 through equations (6.47), (E.83), (E.84), and (E.85). They are needed to describe the dependency on the saturation of oil and water. The closure equation (E.86) constitutes an algebraic constraint together with $\mathbf{p}^w = \mathbf{p}^o$ which is already integrated in the set of equations. The reservoir simulations performed in this work are based on an implementation of the model equations (6.40) - (6.47) in MATLAB[2]. The source code SIMSIM[3] was used as a basis for the simulations that were carried out.

Tellegen's Theorem for Two-phase Flow

Tellegen's theorem for oil-water-flow is given as

$$(\frac{\mathbf{p}}{\rho^w})^T \frac{d\mathbf{M}^w}{dt} = -(\frac{\Delta\mathbf{p}}{\rho^w})^T \dot{\mathbf{M}}^{\mathbf{w}} - (\frac{\mathbf{p_Q}}{\rho^w})^T \mathbf{Q}^w \tag{6.48}$$

$$(\frac{\mathbf{p}}{\rho^w})^T \frac{d\mathbf{M}^o}{dt} = -(\frac{\Delta\mathbf{p}}{\rho^w})^T \dot{\mathbf{M}}^{\mathbf{o}} - (\frac{\mathbf{p_Q}}{\rho^w})^T \mathbf{Q}^o \tag{6.49}$$

The term of the left hand side is an accumulation term $(\frac{\mathbf{p}}{\rho^{o,w}})^T \frac{d\mathbf{M}^{o,w}}{dt}$ for the storage of potential energy in the grid cells. On the right hand side, there are two terms for in- and outflux of power: Resistive terms for the energy dissipation through percolation of the fluid $(\frac{\Delta\mathbf{p}}{\rho^{o,w}})^T \dot{\mathbf{M}}^{\mathbf{o,w}}$ and power input/output through the wells $(\frac{\mathbf{p_Q}}{\rho^{o,w}})^T \mathbf{Q}^{o,w}$.

If we assume constant density for each liquid phase, we have

$$\mathbf{p}(t_1)^T V\phi \frac{d\mathbf{S}^w(t_2)}{dt} + (\mathbf{p}(t_1)^T V\mathbf{S}^w(t_2))^T \phi(\mathbf{c}^r + \mathbf{c}^w)\frac{d\mathbf{p}(t_2)}{dt} = -\mathbf{p}^T(t_1)\mathbf{T}^{\mathbf{w}}\mathbf{p}(t_2) - \mathbf{p_Q}^T(t_1)\mathbf{Q}^w(t_2) \tag{6.50}$$

$$\mathbf{p}(t_1)^T V\phi \frac{d\mathbf{S}^o(t_2)}{dt} + (\mathbf{p}(t_1)^T V\mathbf{S}^o(t_2))^T \phi(\mathbf{c}^r + \mathbf{c}^o)\frac{d\mathbf{p}(t_2)}{dt} = -\mathbf{p}^T(t_1)\mathbf{T}^{\mathbf{o}}\mathbf{p}(t_2) - \mathbf{p_Q}^T(t_1)\mathbf{Q}^o(t_2) \tag{6.51}$$

For $t_1 = t_2$ Tellegen's Theorem results in an instantaneous power balance which is given in summation

[2]MATLAB is a numerical computing environment and programming language.

[3]SIMSIM is a reservoir simulation code developed at the TU Delft by Jan Dirk Jansen. Jan Dirk Jansen is with the faculty of Civil Engineering and Geosciences.

form as

$$\sum_{i=1}^{n_p}(p_i V\phi_i\frac{dS_i^w}{dt}+p_i VS_i^w(c^r+c^{w,o})\phi_i\frac{dp_i}{dt}) = -\sum_{FLOWS}\Delta p_{ij}\dot{V}_{ij}^w + \sum_{WELLS}(p_{well,i}-p_i)\dot{Q}_i^w+\sum_{INJ}p_{well,i}\dot{Q}_i^w-\sum_{PROD}p_{well,i}\dot{Q}_i^w \tag{6.52}$$

$$\sum_{i=1}^{n_p}(p_i V\phi_i\frac{dS_i^o}{dt}+p_i VS_i^o(c^r+c^{w,o})\phi_i\frac{dp_i}{dt}) = -\sum_{FLOWS}\Delta p_{ij}\dot{V}_{ij}^o + \sum_{WELLS}(p_{well,i}-p_i)\dot{Q}_i^o+\sum_{INJ}p_{well,i}\dot{Q}_i^o-\sum_{PROD}p_{well,i}\dot{Q}_i^o \tag{6.53}$$

Tellegen's theorem holds if the two Kirchhoff laws apply to the regarded model and states that the potential variables and the flow variables span orthogonal spaces. The principle holds true even if we regard potentials from a particular state at time t_1 and flows from a particular state t_2.

Dissipative and Passive Properties of Two-phase Flow

Definition 17. *The petroleum reservoir is said to be dissipative with respect to the supply rate* $\phi_E(\dot{\mathbf{V}}_\mathbf{T},\mathbf{p}_\mathbf{T})$*, if there exists a storage function* $E(\mathbf{V}^o,\mathbf{V}^w)$ *so that for all* $t\geq 0$*, all initial conditions and all controls*

$$0\leq E(\mathbf{V}^o(t),\mathbf{V}^w(t))\leq E(\mathbf{V}^o(0),\mathbf{V}^w(0))+\int_0^t\phi_E(\dot{\mathbf{V}}_\mathbf{T},\mathbf{p}_\mathbf{T})$$

The dissipation inequality expresses the fact that the stored energy does not increase beyond supply plus initial storage.

Definition 18. *A dissipative subsurface flow process with input vector* $\dot{\mathbf{V}}_\mathbf{T}$ *or* $\mathbf{p}_\mathbf{T}$ *and output vector* $\mathbf{p}_\mathbf{T}$ *or* $\dot{\mathbf{V}}_\mathbf{T}$ *is passive, if there exist non-negative constants* β_i *so that the supply rate is written*

$$\phi_E(\dot{\mathbf{V}}_\mathbf{T},\mathbf{p}_\mathbf{T}) = \mathbf{p}_\mathbf{T}{}^T\mathbf{F}_\mathbf{T}-\beta_1\dot{\mathbf{V}}_\mathbf{T}^T\dot{\mathbf{V}}_\mathbf{T}-\beta_2\mathbf{p}_\mathbf{T}{}^T\mathbf{p}_\mathbf{T}$$

Theorem 28. *A reservoir is considered passive, if the constitutive equations are positive and*

$$\frac{\partial E}{\partial \mathbf{V}^o}\mathbf{A}\dot{\mathbf{V}}^o + \frac{\partial E}{\partial \mathbf{V}^w}\mathbf{A}\dot{\mathbf{V}}^w \leq \mathbf{p_T}^T\mathbf{F_T} - \beta_1\dot{\mathbf{V}}_\mathbf{T}^T\dot{\mathbf{V}}_\mathbf{T} - \beta_2\mathbf{p_T}^T\mathbf{p_T} \tag{6.54}$$

Proof. See App. E.9. □

Darcy's law for flow of liquids in porous rock is positive in the passivity sense, i.e., reservoir flow through porous rock is dissipative and it follows that the system converges asymptotically to a stable steady state. It is important to note that the vectors $\dot{\mathbf{V}}_\mathbf{T}$ and $\mathbf{p_T}$ represent the flows and pressures at the terminals, i.e., the wells. For a passive system, the controls and measurements have to be chosen in particular input-output pairs. e.p., if the pressure at a certain well is controlled then the flow has to be measured and vice versa.

6.2 Variational Principles

The dissipation function $\sigma = \sum_i \dot{V}_i \Delta p_i$ as introduced in Chapter 3, eq. (3.9) and describes the heat produced through viscous friction in the reservoir and serves as a metric for the potential gradients in the system. The dissipation function for the reservoir can be decomposed into the content and cocontent of the reservoir as derived in Chapter 3 as in

$$\sigma(\dot{\mathbf{V}}, \Delta\mathbf{p}) = G^*(\Delta\mathbf{p}) + G(\dot{\mathbf{V}}) \tag{6.55}$$

where the content G and cocontent G^* are Legendre-transforms of one another.

6.2.1 Pressure Dynamics

For a single-phase reservoir with weakly compressible behavior and constant pressures at the terminals, we derive a potential function based on the gridblock pressures as dynamic variables integrating

the cocontent

$$\min_{\mathbf{p}} \quad G^* = \int_0^{\Delta \mathbf{p}} \dot{\mathbf{V}}^T d(\Delta \mathbf{p}) \tag{6.56}$$

$$s.t. \qquad \Delta \mathbf{p} = \mathbf{A^T p} \tag{6.57}$$

$$\dot{\mathbf{V}} = \frac{h}{\mu} k \Delta \mathbf{p} \tag{6.58}$$

$$\mathbf{p_Q} = \text{const} \tag{6.59}$$

analogously to the derivation of the potential function in Chapter 3, we derive

$$\Psi(\mathbf{p}) = \frac{1}{2} \mathbf{p}^T \Phi \mathbf{p} \tag{6.60}$$

This potential function is a quadratic form where

$$\Phi = \begin{bmatrix} \mathbf{A_x T_x A_x}^T & \mathbf{0} \\ \mathbf{0} & \mathbf{A_y T_y A_y}^T \end{bmatrix}$$

The dynamics can be written out as a gradient system

$$V c_t \phi \frac{d\mathbf{p}}{dt} = \frac{\partial \Psi}{\partial \mathbf{p}} \tag{6.61}$$

with $\frac{\partial \Psi}{\partial \mathbf{p}}$ being a gradient vector field of the $\mathbb{C}^2$ function $\Psi(\mathbf{p})$. It can easily be verified that the function $\Psi(\bar{\mathbf{p}})$ is a strict Lyapunov function in some neighborhood of $\mathbf{p}^*$, where $\bar{\mathbf{p}} = \mathbf{p} - \mathbf{p}^*$. It follows that $\mathbf{p}^*$ is an asymptotically stable equilibrium point for the gradient system (6.61). The state trajectory of the single-phase reservoir follows the path of steepest descent on the hypersurface of the potential function, i.e., at regular points, the vector field $\frac{\partial \Psi}{\partial \mathbf{p}}$ is perpendicular to the level surface of $\Psi(\mathbf{p})$. In case of weakly compressible flow, a quadratic potential function results which is globally convex. Nonregular points are hence equilibria of the system, where isolated minima

are asymptotically stable [20]. Fig. 6.2 shows a simulation of a simple six grid block reservoir (see App. E.5.1) during injection. The injection and production rates converge into a steady state. Simultaneously, the dissipation converges to the minimum of $\Psi(\mathbf{p})$ in around 1000 days

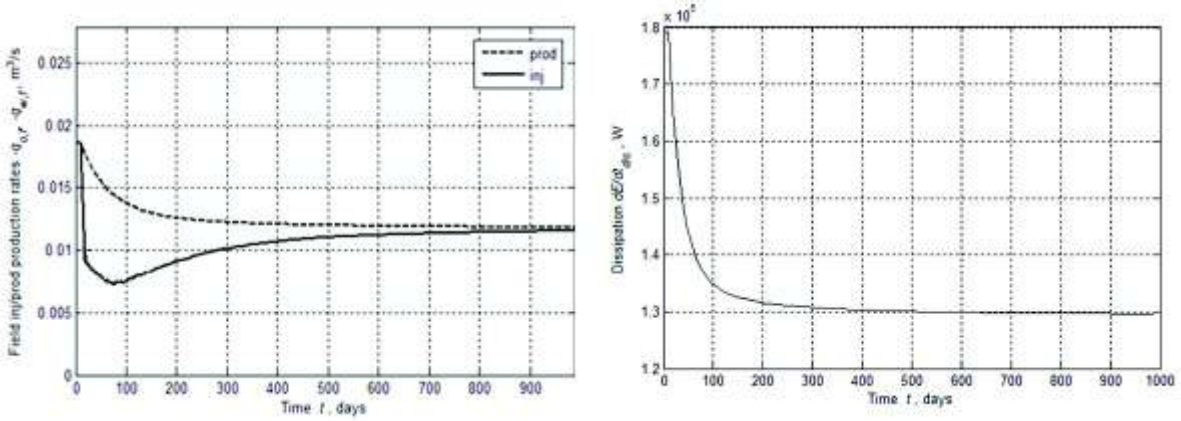

Figure 6.2: Production, injection rate, and dissipation for the six grid block single phase example.

To analyze the connection between the dissipative behavior of the reservoir and the water injection process, we extend the model to a two-phase oil water system. Our theory regards the reservoir as a system consisting of two coupled flow networks for each component, see Fig. 6.3. An important

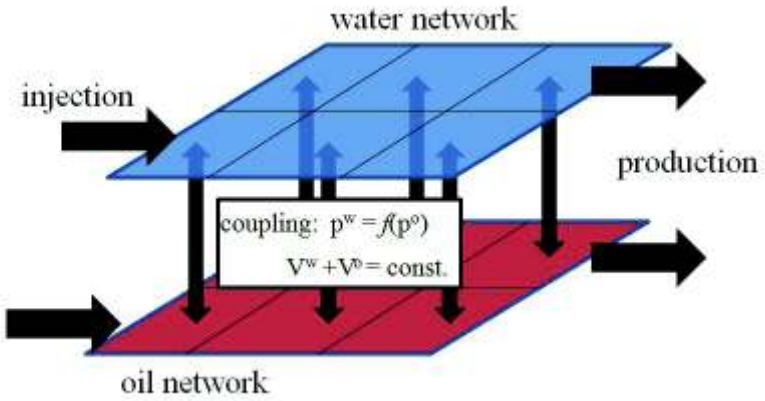

Figure 6.3: Petroleum reservoir from a network perspective.

aspect considered for dissipative flow networks with multiple phases is a change in the degrees of

freedom due to the coupling of intensive and extensive variables. Reversible processes are coupled in their intensive variables, i.e., a subsystem that is considered in thermodynamic equilibrium has equal temperature, pressure, and chemical potentials across different phases. For the reservoir, each gridcell is a system at thermodynamic equilibrium with uniform pressure for both phases. Further, the gridblock volume is constant and the oil and water phase share the total available pore volume given through the equation $V_i^w + V_i^o = V_i^{total}$. The coupling of the water and oil network leads to an increase in the degrees of freedom of the pressures at the boundaries (wells) as compared to the single-phase network. The single-phase network requires the specification of one flow or pressure per well, resulting in a total of n_T variables that have to be specified. In case of the two-phase reservoir, the specification of n_T flows or potentials at the wells is necessary in addition to the ratio of water and oil at the injection wells.

The reservoir solves two separate but interdependent optimization problems for the water network

$$\min_{\mathbf{p^w}} \quad J^w = \int_0^{\Delta \mathbf{p^w}} (\dot{\mathbf{V}}^{\mathbf{w}})^T d(\Delta \mathbf{p^w}) \tag{6.62}$$

$$s.t. \qquad \Delta \mathbf{p^w} = \mathbf{A^T p^w} \tag{6.63}$$

$$\dot{\mathbf{V}}^{\mathbf{w}} = \tfrac{h}{\mu} k \Delta \mathbf{p^w} \tag{6.64}$$

$$\mathbf{p_Q^w} = \text{const} \tag{6.65}$$

and the oil network

$$\min_{\mathbf{p^o}} \quad J^o = \int_0^{\Delta \mathbf{p^o}} (\dot{\mathbf{V}}^{\mathbf{o}})^T d(\Delta \mathbf{p^o}) \tag{6.66}$$

$$s.t. \qquad \Delta \mathbf{p^o} = \mathbf{A^T p^o} \tag{6.67}$$

$$\dot{\mathbf{V}}^{\mathbf{o}} = \tfrac{h}{\mu} k \Delta \mathbf{p^o} \tag{6.68}$$

$$\mathbf{p_Q^o} = \text{const} \tag{6.69}$$

which are connected through

$$\mathbf{S^o} + \mathbf{S^w} = 1 \tag{6.70}$$

$$\mathbf{p^o} = \mathbf{p^w} \tag{6.71}$$

Additivity of both optimization problems gives the following optimization problem:

$$\min_{\mathbf{p^w},\mathbf{p^o}} \quad J = \int_0^{\Delta \mathbf{p^w}} (\dot{\mathbf{V}}^{\mathbf{w}})^T d(\Delta \mathbf{p^w}) + \int_0^{\Delta \mathbf{p^o}} (\dot{\mathbf{V}}^{\mathbf{o}})^T d(\Delta \mathbf{p^o}) \tag{6.72}$$

$$s.t. \qquad \Delta \mathbf{p^w} = \mathbf{A^T p^w} \tag{6.73}$$

$$\Delta \mathbf{p^o} = \mathbf{A^T p^o} \tag{6.74}$$

$$\dot{\mathbf{V}}^{\mathbf{w}} = \tfrac{h}{\mu} k \Delta \mathbf{p^w} \tag{6.75}$$

$$\dot{\mathbf{V}}^{\mathbf{o}} = \tfrac{h}{\mu} k \Delta \mathbf{p^o} \tag{6.76}$$

$$\mathbf{p^w_Q} = \text{const} \tag{6.77}$$

$$\mathbf{p^o_Q} = \text{const} \tag{6.78}$$

$$\mathbf{S^o} + \mathbf{S^w} = 1 \tag{6.79}$$

$$\mathbf{p^o} = \mathbf{p^w} \tag{6.80}$$

For two-phase flow, the potential function, as a function of pressure, is found by integrating the cocontent for water and oil flow:

$$\Psi(\mathbf{S}, \mathbf{p}) = \frac{1}{2} \mathbf{p}^T \Phi^w(\mathbf{S}^w) \mathbf{p} + \frac{1}{2} \mathbf{p}^T \Phi^w(\mathbf{S}^o) \mathbf{p} \tag{6.81}$$

where

$$\Phi^{o/w} = \begin{bmatrix} \mathbf{A_x T_x^{o/w}}(\mathbf{S}) \mathbf{A_x}^T & \mathbf{0} \\ \mathbf{0} & \mathbf{A_y T_y^{o/w}}(\mathbf{S}) \mathbf{A_y}^T \end{bmatrix}$$

The dynamic term for the saturations in the constitutive equations is eliminated by adding (6.38) and

(6.39) resulting into $V\Phi\mathbf{c}(\mathbf{S})\frac{d\mathbf{p}}{dt}$ as the term for the left hand side of the differential equation system with $\mathbf{c} = (\mathbf{c^r} + \mathbf{S^{w}}^T\mathbf{c^w} + \mathbf{S^{o}}^T\mathbf{c^o})$ (see also App. E.4 for details). The pressure dependent dynamic behavior can be described by the gradient system

$$V\Phi\mathbf{c}(\mathbf{S})\frac{d\mathbf{p}}{dt} = \frac{\partial\Psi(\mathbf{S},\mathbf{p})}{\partial\mathbf{p}} \tag{6.82}$$

The pressure dynamics is described by the gradient system of (6.82) with an additional variables given through the saturations $\mathbf{S}$. The saturations serve as a set of parameters for (6.82), since they are not described through a differential term. For the description of the saturation dynamics, we now derive the advective dynamics for the oil-water distribution in the reservoir.

6.2.2 Saturation Dynamics

For the saturation as primary variable, we can identify a set of variables and fundamental equations similar to the one given for the pressures as can be seen in Fig. 6.4. For the saturation dynamics, we choose to study a first order problem, namely, equal viscosity and first-contact miscible displacement in two dimensions, and in the absence of dispersion and gravity. Similar to the pressure dynamics,

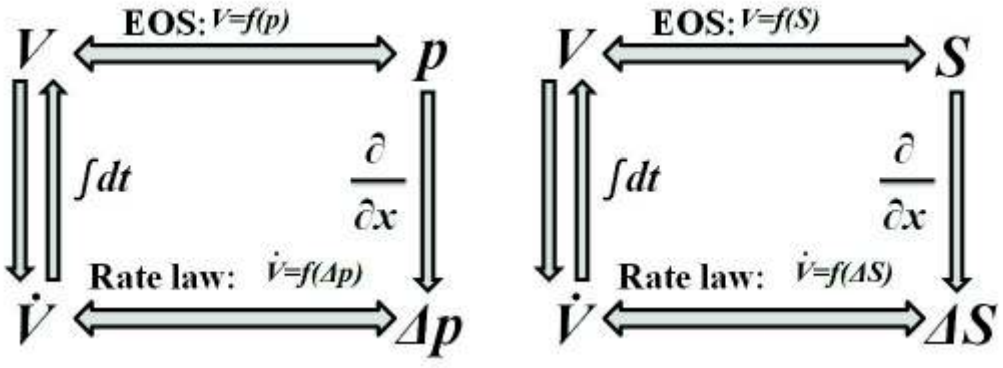

Figure 6.4: Relevant sets of dynamic variables and their mathematical connections.

we define the saturation as a potential with the following capacitive constitutive equation:

$$\mathbf{S} = \frac{1}{V}\mathbf{V^w} \tag{6.83}$$

and a constitutive law for resistive flow

$$\dot{\mathbf{V}}^{\mathbf{w}} = \Delta \mathbf{p}^T \frac{\mathbf{k}}{\mu} \Delta \mathbf{S} \tag{6.84}$$

where we assume equal water and oil viscosity $\mu = \mu^w = \mu^o$ and linear relative permeability. The resistive constitutive equation is adapted from Darcy's law, in which flow of water only leads to change in saturation of the connected gridcells for $\Delta \mathbf{S} \neq 0$. The pressure serves as a parameter similar to the saturation in (6.82) which can be considered constant, slowly varying, or dynamic dependent on the differential system for the pressure.

The product $\sigma = \sum_i \dot{V}_i^w \Delta S_i^w$ defines dissipation for the combination of volume V^w and saturation S^w. The dissipation is here an artificial quantity that does not directly relate to an energetic function. The saturation dynamics are considered advectively coupled to the diffusive properties of the pressure dynamics. The saturation cocontent G_S^* for a reservoir with constant pressure $\mathbf{p_Q}$ at all wells and fixed saturation $\mathbf{S_{Q,inj}}$ at the injection wells, i.e., injection of water:

$$G_S^* = \int_0^{\Delta \mathbf{S}} (\dot{\mathbf{V}}^{\mathbf{w}})^T d(\Delta \mathbf{S}) \tag{6.85}$$

Using (6.84), we derive the potential function

$$\Psi^S(\mathbf{S}) = \frac{1}{2} \Delta \mathbf{S}^T \frac{\mathbf{k} \Delta \mathbf{p}}{\mu} \Delta \mathbf{S} \tag{6.86}$$

The drift equation for the saturation is found by differentiating the potential function (6.86)

$$V\Phi\frac{d\mathbf{S}}{dt} = \frac{\partial\Psi^S(\mathbf{S},\mathbf{p})}{\partial\mathbf{S}} \tag{6.87}$$

which gives

$$V\Phi\frac{d\mathbf{S}}{dt} = \Delta\mathbf{p}^T\frac{\mathbf{k}}{\mu}\Delta\mathbf{S} \tag{6.88}$$

The relative permeability accounts for the increased resistance of flow for one liquid in a pore wetted by another liquid. This behavior is taken into account through the pressure potential function, where the resistivity is saturation dependent. Pressure gradients in turn change dependent on saturation and result in changes of resistance in the saturation potential function. This behavior leads to the coupled dynamic system described by

$$V\Phi\mathbf{c}(\mathbf{S})\frac{d\mathbf{p}}{dt} = \frac{\partial\Psi(\mathbf{S},\mathbf{p})}{\partial\mathbf{p}} \tag{6.89}$$

$$V\Phi\frac{d\mathbf{S}}{dt} = \frac{\partial\Psi^S(\mathbf{S},\mathbf{p})}{\partial\mathbf{S}} \tag{6.90}$$

Example 4. *To demonstrate the injection process and its connection to the potential function behavior, we investigate the waterflooding process of a typical petroleum field case study. The case study we consider [7] is a heterogeneous, 2D, two-phase (oil/water) reservoir with two horizontal smart wells, an injector and a producer, at opposite sides, see Fig. 6.5. The reservoir has no-flow boundaries at all sides. Each well is divided into segments with inflow control valves, allowing for individual inflow control of the segments. Alternatively, the two horizontal wells can be seen as rows of vertical injectors and producers. For the particular setup, we inject water through the injectors on the left hand side and produce a 2-phase mixture of oil and water on the right hand side of Fig 6.5. The simulation and optimization can either be flow rate controlled or pressure controlled at the injector and producer wells. We assume a permeability field for the 2D reservoir based on [7], see*

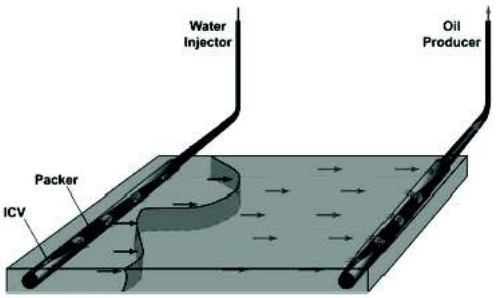

Figure 6.5: Schematic of waterflooding in reservoir with a horizontal smart injector located along the left edge, and a smart producer along the right edge from [7].

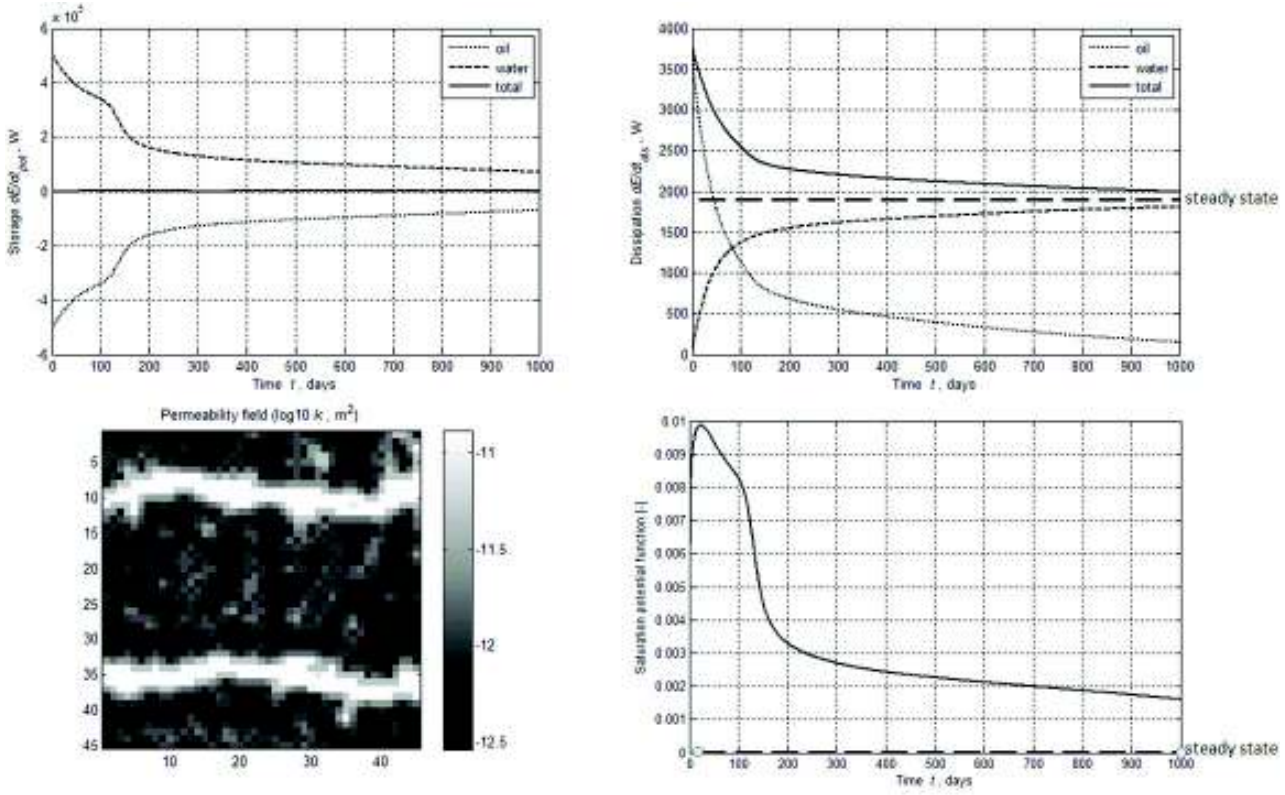

Figure 6.6: Stored potential energy in reservoir (top left), dissipated energy (top right), permeability field with two low permeability streaks (bottom left), and potential function for saturation behavior (bottom right).

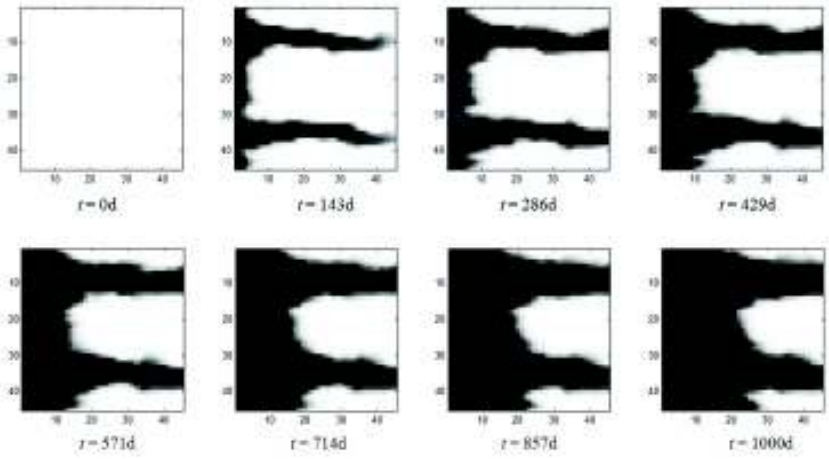

Figure 6.7: Time sequence of reservoir during water (black) injection where oil (white) is moved and produce on the right hand side.

Fig. 6.6, bottom left. The parameters are given in App. E.5.2 and model equations are given by the DAE system in Section 6.1.3. Fig. 6.6 illustrates the change of the dissipation function $\Psi(\mathbf{p},\mathbf{S})$ *as a function of time in the top right graph, while the change of potential energy is shown in the top left graph. The top left figure illustrates that during a brief initial period potential energy is released from the reservoir through oil flow, but that an equilibrium is rapidly established during which the total amount of potential energy stored stays nearly constant and close to zero. The dissipation in the top right figure caused by oil flow reduces with time while the dissipation caused by water flow increases, corresponding to the increasing water-oil ratio of the produced reservoir fluids. The total dissipation in the reservoir decreases reaching the minimum expected for the dissipation function* $\Psi(\mathbf{p},\mathbf{S})$*. The bottom right graph shows the saturation potential function decrease which reaches a minimum once all of the movable oil is produced. The time plot in Fig. 6.7 shows how water (black) subsequently pushes oil (white) out of the reservoir while two distinct high permeability streaks develop.*

6.3 Implications on Displacement Efficiency

The objective in reservoir management is to maximize the volume of recovered oil from the reservoir over a certain time horizon T

$$\max \Phi = \sum_{PROD} \int_{t=0}^{T} \dot{Q}_i^{o,PROD} dt \tag{6.91}$$

subject to operational constraints such as flow capacity and pressure limits at the injection and production wells. A formulation for a common closed loop optimization strategy is given in App. E.10. The time horizon is subject to the profitability condition, i.e., at the end of the time horizon, the operations balance becomes negative. The total oil balance for the reservoir

$$\sum_{i=1}^{n_{GB}} \frac{dV_i^o}{dt} = - \sum_{PROD} \dot{Q}_i^{o,PROD} \tag{6.92}$$

with objective (6.91) gives the following

$$\min \Phi = \sum_{i=1}^{n_{GB}} \int_{t=0}^{T} \frac{dV_i^o}{dt} dt = \sum_{i=1}^{n_{GB}} V_i^o(T) \tag{6.93}$$

which is still given in terms of volume of oil. A common formulation in reservoir engineering is the use of the water saturation S^w as parameter which can be obtained as

$$\max \Phi = \sum_{i=1}^{n_{GB}} \int_{t=0}^{T} \frac{dS_i^w}{dt} dt = \sum_{i=1}^{n_{GB}} S_i^w(T) \tag{6.94}$$

If we use the proportionality from (6.88)

$$\frac{d\mathbf{S}}{dt} \propto \Delta \mathbf{p}^T \frac{\mathbf{k}}{\mu} \Delta \mathbf{S}$$

it follows

$$\max \Phi = \sum_{i=1}^{n_{FLOWS}} \int_{0}^{T} \Delta p_i \frac{k_i}{\mu} \Delta S_i dt \tag{6.95}$$

Eq. (6.95) provides an important insight. It shows that the most effective strategy is found for the pressure gradients being largest at the location of the largest saturation gradients. In a production setting with limited energy input into the reservoir, the energy should be distributed among the wells as to maximize the pressure gradients at the water-oil front throughout injection. We can also infer that the steeper the gradients the faster the recovery, which applies to both pressure and saturation gradients.

6.3.1 Injection Principles

We pose the problem as an integrated platform and oil field, to analyze the displacement of oil from a thermodynamic viewpoint. Limited resources of energy are available through the injector pumps at an oil reservoir. The control valves for the producers allow the reduction of flow in the production wells. The design of the platform and its components is fixed and it is given from previous production activities during the first recovery stage. Fig. 6.8 shows integrated oil field and platform for a basic case study with 4 injectors and 9 producers. The example is used to illustrate the principles from previous theoretical derivations in a practical setting.

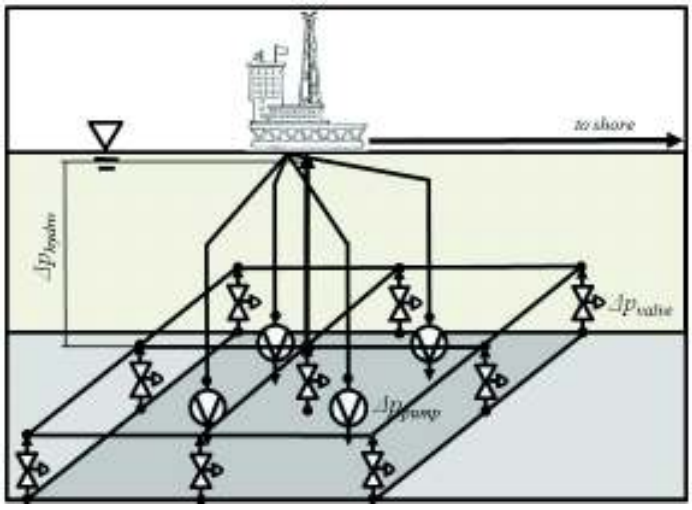

Figure 6.8: Schematic of a square reservoir with 4 injectors and 9 producers connected to periphery including platform.

Petroleum fields in the second recovery stage consist of an arrangement of wells that have previously produced oil driven by the natural pressure of the reservoir. Some of the production wells are converted into injection wells and water is injected into the reservoir to produce the remaining oil. We assume smart injection wells with measurements of liquid flow and bottomhole pressure. The pumping power of the injectors and the pressure drop across the producer valves serve as control variables. Since our focus is on the dissipative properties of the reservoir, we ignore hydrostatic effects in the vertical pipelines connecting the subsea arrangement to the surface facilities. Generally, these hydrostatic forces caused by density differences between injected water and produced hydrocarbons create an additional lifting force naturally enhancing the production flow.

Fig. 6.9 shows the reservoir with 4 injectors and 9 producers from the top view (left) and a network representation (right). The abstraction of the petroleum reservoir as a resistive network in

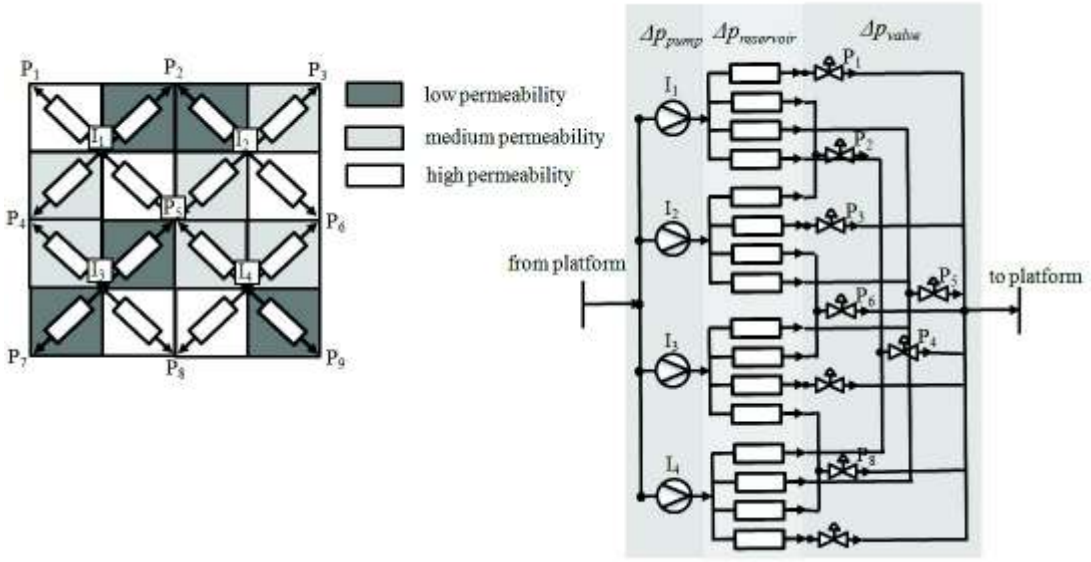

Figure 6.9: Schematic of a square reservoir with 4 injectors and 9 producers and sectors of varying permeability represented by resistances (left) and network representation using terminals and flow connections (right).

Fig. 6.9 shows several important principles. Firstly, the reservoir consists of four arrangements of inverted five spots, i.e., four production wells are arranged around each one of the four injectors I_1,

I_2, I_3, and I_4. Dependent on the geometrical shape of the reservoir, different patterns ranging from (inverted) two-spot to (inverted) nine-spot arrangements with a single production or injection well in the center of a "circle" of wells exist. We assume the field can be subdivided into elementary 3- to 5-spots or their inverted counterparts, see Fig. 6.10. Most fields of different shapes and geology contain well patterns that can be decomposed into elementary elements. As can be seen in Fig. 6.10, some of the production wells are shared between different elementary 5-spots such as for example Producer P_2. The elementary five spot in the center shares the center producer P_5 with all four inverted five spots. The complexity in designing a good injection strategy lies here in managing the decomposition of decision making into decentralized policies that still account for the cooperation necessary for the shared wells of adjacent elementary 5-spots.

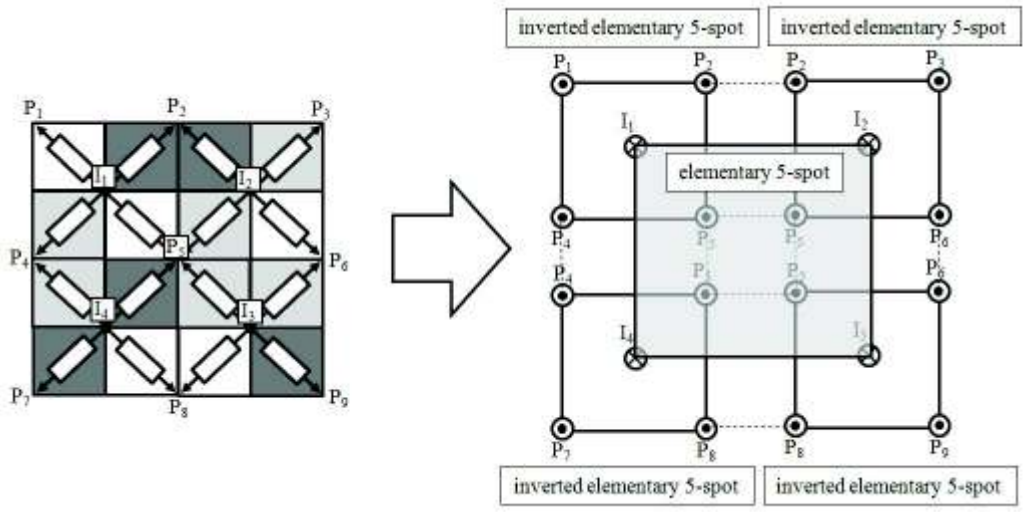

Figure 6.10: Schematic of a square reservoir with 4 injectors and 9 producers and sectors decomposed into elementary five spots and inverted five spots (right).

Definition 19. *An injection strategy is considered optimal with respect to oil recovery and profits from oil recovery, if the energy output from the injectors is maximized, the resistance of the platform-oil field development is minimized, and the ratio of energy dissipation through movement of oil versus movement of water is maximized over the production horizon.*

From the Definition 19, we derive four elementary principles for the injection strategy.

1. **Maximize Selectivity**: The dissipation of energy in the reservoir should be distributed such that a maximum of energy is used to move oil towards the production wells while energy losses through water production are minimized.

2. **Minimize valve resistance**: The energy dissipated through valve resistances should be minimized, i.e., the valves should be operated fully open or fully closed with minimum transition times between the two possible states (bang-bang control).

3. **Maximize energy input**: The amount of energy injected into the reservoir through the injector pumps should be maximized.

4. **Maximize profitability and discounting**: Oil in high permeability regions should be produced before oil in low permeability regions of the reservoir for higher operational profits due to discounting and operational production costs.

The first two principles address the displacement efficiency from a technical point of view stating that for a given injector input, energy losses through water production and valve choking should be kept at a minimum. The remaining two principles address rather the economic component of the displacement efficiency. There exist infinite different strategies that are technically optimal according to the first two principles, but vary in economic efficiency, i.e., although energy is used at maximum efficiency, slower production can lead to extended production horizons and hence suboptimal operation. From the economic objective regarding operations costs, depreciation of equipment and discounting, it is important to recover oil as fast as possible. In the following, we address these principles separately based on the dissipative properties during the injection process.

Principle 1: Minimization of water production

Definition 20. *We define the internal efficiency*

$$\eta^{int} = \frac{\mu^w}{\mu^0}\frac{\sigma^o}{\sigma^w} \tag{6.96}$$

to achieve a given recovery factor q with $0 \leq q \leq 1$ of a displacement process, where

$$\sigma^o = \int_0^{T^{90}} \sum_{i=1}^{n_{FLOWS}} \dot{V}_i^o \Delta p dt$$

is the dissipation caused through movement of oil and

$$\sigma^w = \int_0^{T^{90}} \sum_{i=1}^{n_{FLOWS}} \dot{V}_i^w \Delta p dt$$

the dissipation caused through movement of water. The time horizon to achieve the recovery factor q is defined as

$$T^q = \frac{\int_0^{T^q} \sum_{PROD} \dot{Q}_i^o dt}{V_{total}^o} = q$$

We define the internal efficiency η^{int} as an energy related metric to evaluate the displacement process. The definition of the recovery factor q as a limit for the production horizon is necessary, since full recovery is theoretically and practically impossible due to capillary forces and geological inhomogeneities [3]. During the injection process, the amount of water injected has to be at least the volume of oil stored in the reservoir for the internal efficiency to be a meaningful measure:

$$\int_0^T \sum_{INJ} \dot{Q}_i^w \geq V_{total}^{reservoir} \tag{6.97}$$

Differences in the oil and water dynamic viscosity have been taken into account as a multiplying factor in (6.96). In the following, we assume $\mu^w = \mu^o$. It can be shown that in the limit case of a perfect

oil-water front arriving simultaneously at the production wells, the dissipation through oil flow and the dissipation through water flow are exactly equal such that $\eta^{int} = 1$. The limiting case is illustrated for a line-drive injection process (see also Example 4) of a square reservoir with homogeneous permeability field, see Fig. 6.11. The optimal strategy results from constant and uniform injection and production.

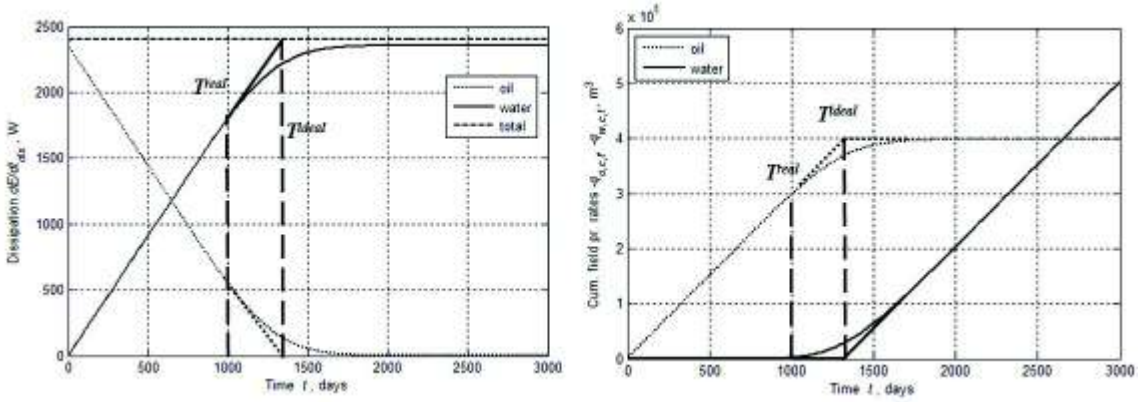

Figure 6.11: On the left, dissipated energy through oil and water flow for a realistic (diffusion of water-oil front) and an idealistic case (no diffusion at water-oil front) of a homogeneous reservoir. The area under the curve, i.e. the dissipated energy, is identical for water and oil dissipation. On the right, the cumulative water and oil production for the realistic and idealized case. The internal efficiency is $\eta^{int}_{ideal} = 1$ for the ideal case and $\eta^{int}_{ideal} = 0.96$ for the diffusive case.

The internal efficiency is a measure of the general displacement efficiency of an injection strategy independent on the injection rates. It correlates with the total recovery and shows a maximum with the strategy that produces the most oil with the least water. Fig. 6.12 shows the internal efficiency in a ternary plot of fractions of total flow rates. Due to the symmetry of the given reservoir, we combine the producers in the medium permeability parts in the northeast and southwest as one fraction and the low permeability streak in the northwest and the high permeability region of the southeast producer as the two remaining fractions. The example shows that optimality occurs for an injection strategy where most of the water is injected along the low permeability streaks in the reservoir. The inhomogeneous distribution of resistances in the reservoir leads to self-redirection of flow such that water

and oil saturation gradients align with pressure gradients. Consequently, the water oil front arrives simultaneously at all producers.

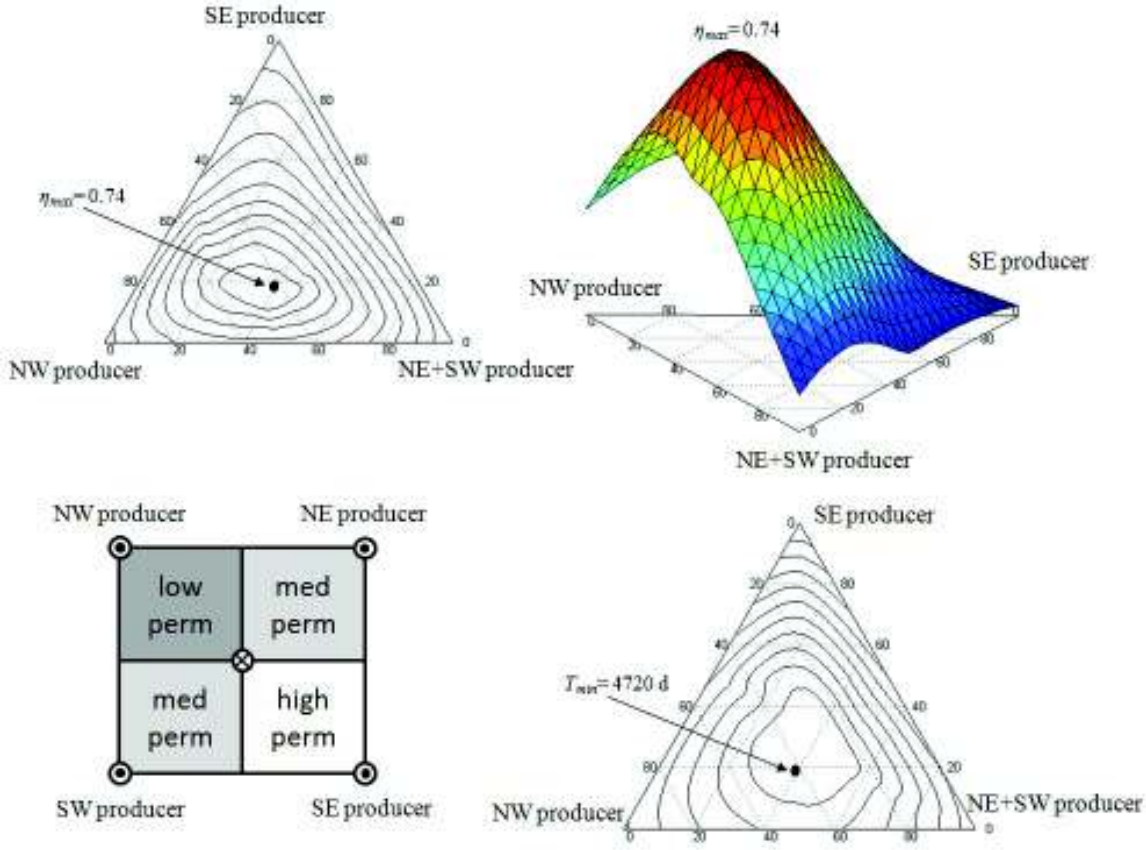

Figure 6.12: Internal efficiency as a function of the fractions of flow through the low permeability northwest producer, the two symmetric medium permeability producers northeast and southwest, and the high permeability producer southeast. The maximum of internal efficiency $\eta_{max} = 0.74$ occurs at fractions of $\frac{\dot{V}_{NW}}{\dot{V}_{total}} = 0.39$, $\frac{\dot{V}_{NE/SW}}{\dot{V}_{total}} = 0.39$, and $\frac{\dot{V}_{NW}}{\dot{V}_{total}} = 0.22$. For the given flow settings the minimum for the 90 % recovery time occurs at the same flow distribution with $T_{min} = 4720$ days.

The maximum for internal efficiency correlates with the minimum time for recovery as can be seen in Fig. 6.12. A theoretical explanation can be derived through the connection between flow related water-oil selectivity and the internal efficiency. The total volume balance of the reservoir is

$$\sum_{i=1}^{n_{GB}} \frac{dV_i^o}{dt} + \sum_{i=1}^{n_{GB}} \frac{dV_i^w}{dt} = \sum_{INJ} \dot{Q}_i^{w,PROD} - \sum_{PROD} \dot{Q}_i^{w,PROD} - \sum_{PROD} \dot{Q}_i^{o,PROD} \tag{6.98}$$

where the left hand side vanishes, since the total liquid volume in the reservoir is considered constant. Assuming the injected water flow as fixed and constant, it follows from (6.98) and (6.91)

$$\max \Phi = \frac{\sum_{PROD} \int_{t=0}^{T} \dot{Q}_i^{o,PROD} dt}{\sum_{PROD} \int_{t=0}^{T} \dot{Q}_i^{w,PROD} dt} \tag{6.99}$$

Using Tellegen's theorem, we determine the total power flux caused by oil and water in the reservoir, where we assume that dynamic changes in pressure occur only in the beginning of the injection period and can be disregarded for most of the injection process for fixed well flow rates

$$\sum_{FLOWS} \Delta p_{ij} \dot{V}_{ij}^{w} = \sum_{INJ} (p_{Q,i}(t_1) \dot{Q}_i^{w} - \sum_{PROD} p_{Q,i} \dot{Q}_i^{w} \tag{6.100}$$

$$\sum_{FLOWS} \Delta p_{ij} \dot{V}_{ij}^{o} = \sum_{PROD} p_{Q,i} \dot{Q}_i^{o} \tag{6.101}$$

Assuming monotonicity between the flow variables $\dot{V}_{ij}^{o,w}$ and the dissipation $\sigma^{o,w}$, it follows that maximizing the internal efficiency is equivalent to (6.99).

Principle 2: Minimization of valve resistance

We introduce the producer efficiency η^{PROD} as an extension of the internal efficiency η^{int} by the efficiency loss $\Delta\eta^{valves} = \frac{\sigma^{valves}}{\sigma^{total}}$ caused by the dissipation of energy through the producer valve resistances

$$\eta^{PROD} = 1 - (1 - \eta^{int}) \frac{\sigma^{w} + \sigma^{o}}{\sigma^{total}} - \frac{\sigma^{valves}}{\sigma^{total}} = 1 - \Delta\eta_{PROD}^{w} - \Delta\eta^{valves} \tag{6.102}$$

$$= \frac{\eta^{int} (\sigma^{w} + \sigma^{o})}{\sigma^{w} + \sigma^{o} + \sigma^{valves}} \tag{6.103}$$

The producer efficiency incorporates the principle of lost energy through control action by choking the producer control valves. In an inverted five spot reservoir as given in Fig. 6.12, we assume that water is injected at the maximum possible rate where the injection pump operates at maximum

power. It is assumed that a minimum pressure p_{rise} is necessary to produce the hydrocarbons from the reservoir depth to the platform. The necessary pressure p_{rise} is a function of the fluid densities of oil and dissolving gas, the pipe resistance, and the pressure at the surface equipment among other factors. Since our focus is on the dissipative properties of the subsurface flow, we assume a constant pressure constraint after the producer valves.

The pressure field can be described using Kirchhoff's voltage law for the pressure, see Fig. 6.10

$$\Delta p_{pump} = \Delta p_{reservoir,i} + \Delta p_{valve,i} \tag{6.104}$$

where $\Delta p_{valve} = p_{bh,i}^{PROD} - p_{rise}$, $\Delta p_{reservoir,i} = p^{INJ} - p_{bh,i}^{PROD}$, $\Delta p_{pump} = p^{INJ} - p^{rise}$. We pose an energy balance based on Tellegen's theorem for the entire reservoir and subsea equipment:

$$\Delta p_{pump} \dot{V}^{INJ,w} = \sum_{FLOWS} \Delta p_{ij} \dot{V}_{ij}^{w} + \sum_{FLOWS} \Delta p_{ij} \dot{V}_{ij}^{o} + \sum_{PROD} \Delta p_{valve,i} \dot{Q}_{i}^{o} + \sum_{PROD} \Delta p_{valve,i} \dot{Q}_{i}^{w} \tag{6.105}$$

or simplified

$$P_{pump} = \sigma^{w} + \sigma^{o} + \sigma^{valves} \tag{6.106}$$

where

$$\begin{aligned} P_{pump} &= \Delta p_{pump} \dot{V}^{INJ,w} \\ \sigma^{o,w} &= \textstyle\sum_{FLOWS} \Delta p_{ij} \dot{V}_{ij}^{o,w} \\ \sigma^{valves} &= \textstyle\sum_{PROD} \Delta p_{valve,i} \dot{Q}_{i}^{o} + \sum_{PROD} \Delta p_{valve,i} \dot{Q}_{i}^{w} \end{aligned}$$

Fig. 6.13 shows the cumulative water and oil production for an injection strategy with all producer valves fully open and shut at a fixed water-to-oil ratio (bang-bang control) versus a strategy with fixed optimized producer settings to maximize the internal efficiency, i.e., minimize water production. In both cases, the power P_{pump} delivered by the injector pump is constant and equal. The bang-bang strategy is completed with the northwest producer shutting down at $t_3 = 4810$ days, see Fig. 6.13 and 6.14.

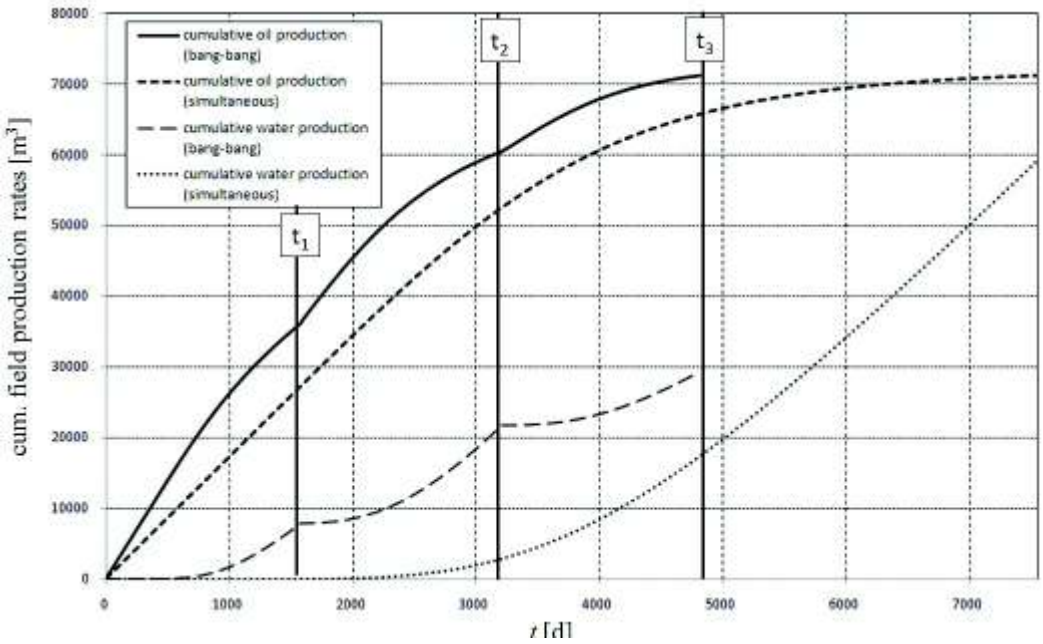

Figure 6.13: Cumulative oil and water production for a bang-bang strategy (solid lines) and a strategy with optimally chosen production rates (dashed lines) for the inverted five spot reservoir from Fig. 6.12. Time t_1 marks the shutting time for the southeast producer at water breakthrough (water ratio cut off $R = 80\%$), t_2 the shutting time for the northeast and southwest producer, and t_3 the shutting time for the northwest producer.

Although the optimized strategy indicates that the energy used for producing oil versus water is optimal, the total available energy delivered by the injector is not used optimally. This can be seen calculating the producer efficiency for the fixed rate strategy $\eta_{fixed}^{PROD} = 0.37$ which is less than the producer efficiency for the bang-bang case $\eta_{bb}^{PROD} = 0.46$. For the bang-bang case, no energy losses occur at the wells due to fully opened or closed valves at all times. The effects of lost energy through well control action can be seen also in the total recovery (Fig. 6.13) where the bang-bang control reaches 98% recovery versus 91% recovery for the case with fixed rates. 98% recovery is reached for the fixed rate strategy only after $t = 7550$ days.

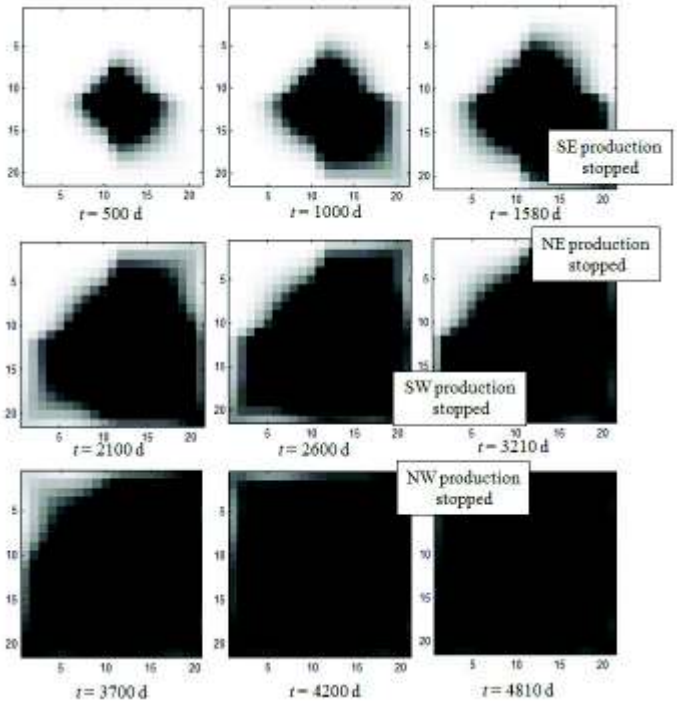

Figure 6.14: Reservoir snapshots for the bang-bang production strategy.

Principle 3: Maximization of Power Input

Similarly to minimizing valve resistance, faster oil recovery is obtained if the injector power input is maximized. We define the injector efficiency as an extension of the internal efficiency

$$\eta^{INJ} = \varphi^{INJ} \eta^{int} \frac{\sigma^w + \sigma^o}{\sigma^{total}} \tag{6.107}$$

where

$$\varphi^{INJ} = \frac{\int^T \sum_{INJ} P_{pump,i}}{\int^T \sum_{INJ} P^{max}_{pump,i}}$$

and $P^{max}_{pump,i}$ is the maximum possible power output of the injector pump i. The cumulative oil and water production of a five spot reservoir with four injectors in the corners and one producer in the center is illustrated in Fig. 6.15. The efficient operation of a five spot reservoir with a single producer in

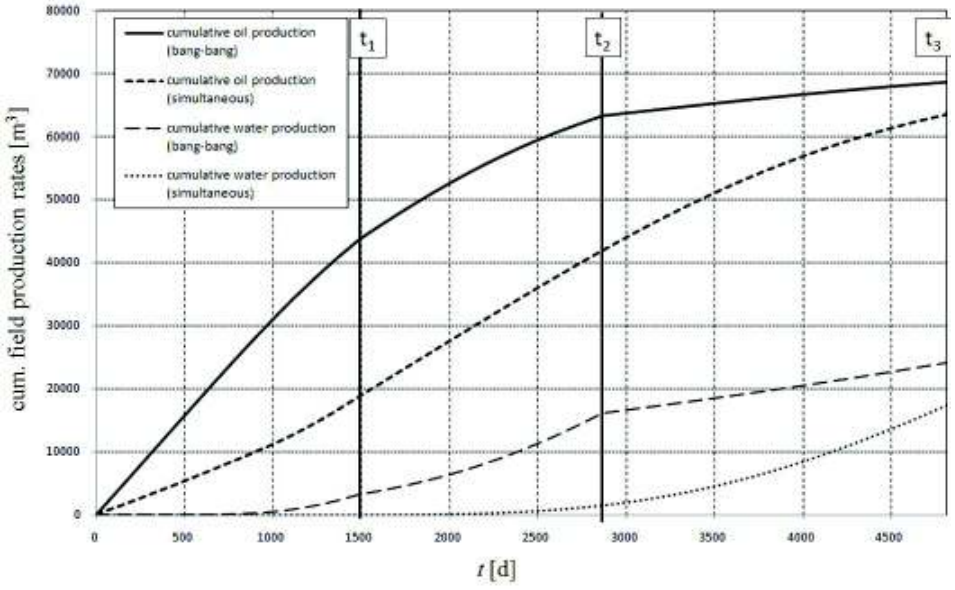

Figure 6.15: Cumulative oil and water production for a bang-bang strategy (solid lines) and a strategy with optimally chosen production rates (dashed lines) for a five spot reservoir identical to Fig. 6.12 with injectors in the corners and a producer in the center. Time t_1 marks the shutting time for the southeast producer at water breakthrough (water ratio cut off $R = 80\%$), t_2 the shutting time for the northeast and southwest producer, and t_3 the shutting time for the northwest producer.

the center is considerably more difficult using strategies limited to information gathered from downhole measurements only. As opposed to the inverted five spot reservoir, the water producing streak of the five spot center producer cannot necessarily be identified and connected to one of the corner injectors without using geological information or tracking technologies. In the simple case of Fig. 6.16, the streak with water breakthrough can be identified based on the measurable pressure gradients and flows. Measurements and permeabilities are not uniquely identifiable if the corner injectors are part of a larger reservoir and injection pattern such that model based data assimilation techniques are necessary. For the bang-bang strategy in Fig. 6.16, injectors were shut down if the amount of water at the center producer surpassed the water-oil ratio of the flow fractions for the respective injectors. The bang-bang strategy recovers more oil compared to the optimized fixed rate strategy but also produces more water. The internal efficiency for the bang-bang strategy was calculated as $\eta_{bb}^{int} = 0.81$ and $\eta_{fixed}^{int} = 0.69$. The bang-bang strategy used $\varphi_{bb}^{INJ} = 0.62$ of the available injection energy compared to $\varphi_{fixed}^{INJ} = 0.36$ which results into a total injector efficiency of $\eta_{bang-bang}^{INJ} = 0.50$ and $\eta_{opt}^{INJ} = 0.25$.

6.3.2 Distributed Injection Strategy

Efficient injection strategies have to obey several principles:

- **Profitability**: Optimality concerning the overall profit of operations.
- **Adaptivity**: Adaptivity to changing conditions in the field, i.e., feedback for the implementation of control to account for disturbances and zero-dynamics.
- **Simplicity**: Minimize control action through robust and simple policies.
- **Efficient data assimilation**: Maximize information content from measurements in the field and at the equipment.

In the following, simple rules for an injection strategy are composed based on the basic principles explained in the previous sections. The strategy assumes the division of the field into elementary

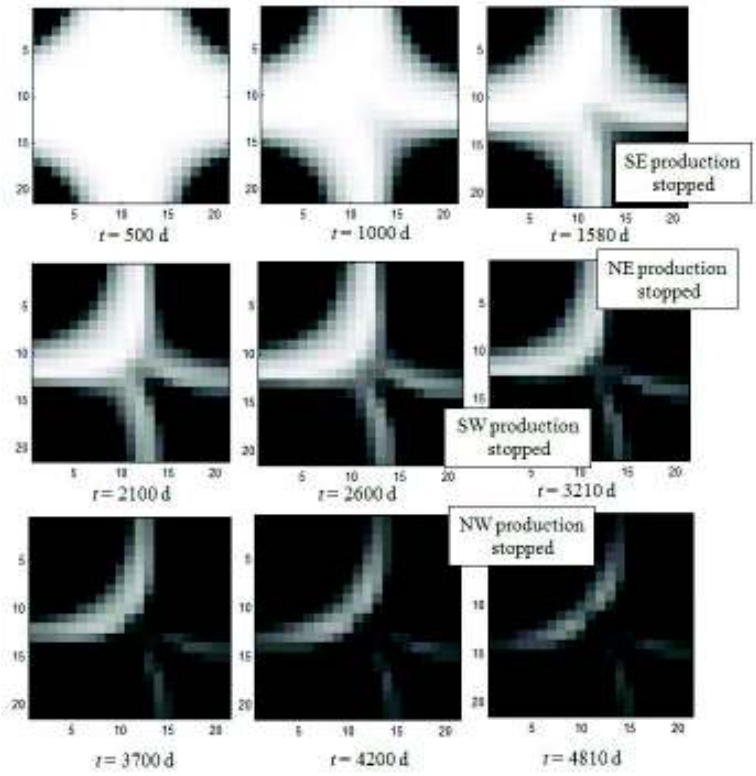

Figure 6.16: Reservoir snapshots for the bang-bang production strategy.

elements most commonly (inverted) five spots:

1. Final shutdown of production wells at a specific water-to-oil ratio typically 80% water and 20% oil (principle 1).

2. Temporary shutdown (principle 1) of a production well at water breakthrough from the direction of a particular injector in close proximity (as part of the elementary five spot surrounding the production well).

3. Production with full injection power (principle 3) and open valves (principle 2). Flow re-directs itself along the path of least resistance and maximizes oil production (principle 4). All injectors and producers are operated in bang-bang mode (principle 2 and 3).

4. Injector shut down if all surrounding production wells are closed.

5. A production well is re-opened after the injector causing the water breakthrough is shut off.

The detection of water breakthrough at a production well along with the identification of the responsible injector can be considered the main technical challenge requiring advanced modeling and control methods. Modern techniques to assist analysis include seismic experiments, chemical and biological analysis of the produced fluids, advanced data assimilation of production data and mathematical modeling and computer algorithms. The mentioned techniques are applied with the aim of understanding how geological properties of the reservoir determine the dynamics of the water oil front, since in most production settings, unnecessary water production occurs due to water breakthrough from one or several high permeability streaks. If information about the permeability field of the reservoir is sufficient, injection strategies can be reduced to very simple procedures such as the policies given above.

In the following example, the injection rules were applied as given above. Water breakthrough is detected for temporary shutdown of producers, if the water fraction in a producer changed in orders

of magnitude in short periods of time, i.e., at the first instance in which water becomes technically ”detectable”. A simple linear resistor analogy (as in 6.9) is used to determine the resistances for each connection between injector and producer in the reservoir based on the bottomhole flow and pressures.

In Fig. 6.17 and 6.18, the strategy is applied to the reservoir of Fig. 6.9. Initial production is started with all producers and injectors open. Subsequently, producers are shut down due to water breakthrough. The corner producers P_1, P_3, P_7, and P_9 are fully open until the water cut is reached. Producers such as P_4, P_5, and P_6 that share fluid influx from different injectors are temporarily shut down and re-opened later to produce the remaining oil once the injector connected to the earlier water breakthrough is shut down. The cumulative oil production for the strategy shows improvement compared to a conventional strategy.

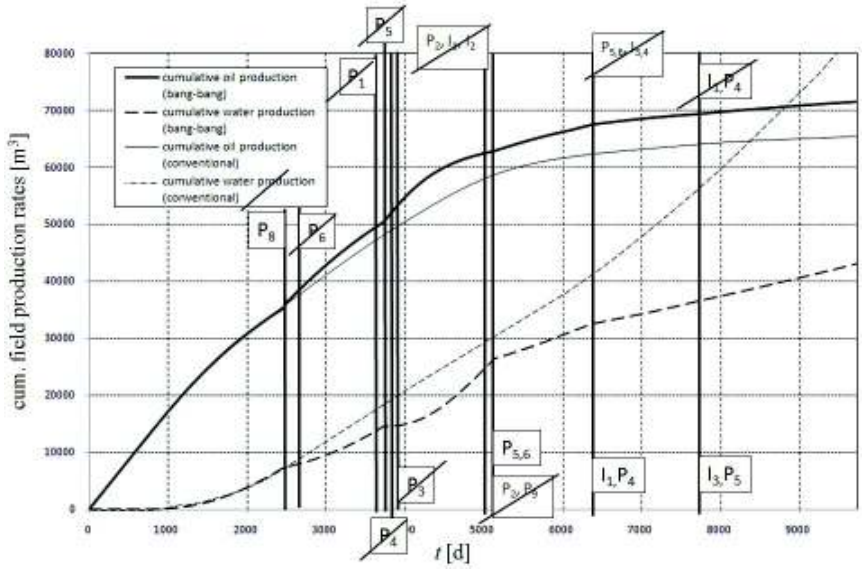

Figure 6.17: Cumulative oil and water production for a distributed injection strategy (solid lines) and a conventional reactive strategy with (dashed lines) for a square reservoir with 4 injectors and 9 producers as in Fig. 6.9. The lines mark a transition point, where injectors and producers are closed or opened.

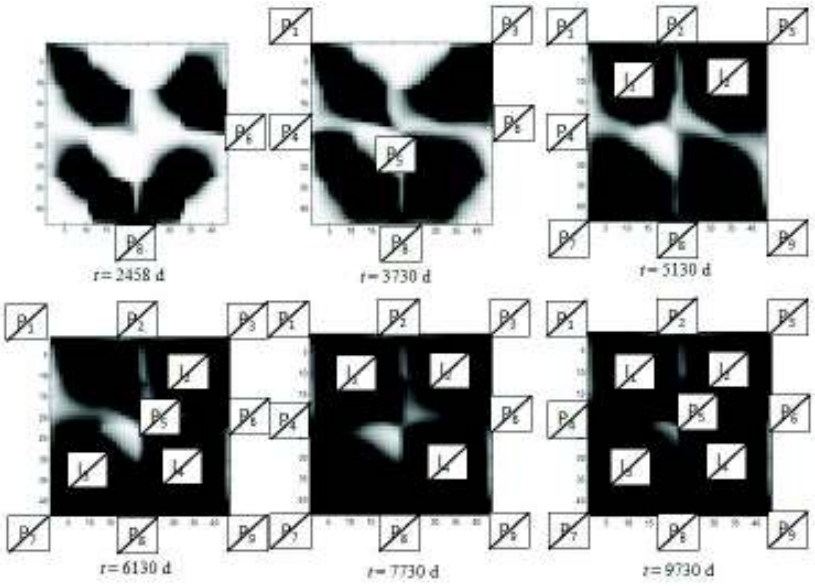

Figure 6.18: Reservoir snapshots for a distributed injection strategy. Closing and opening of producers are indicated through labels.

Chapter 7

Conclusions and Future Directions

”If you don’t know where you are going,
any road will get you there.”
Lewis Caroll

In this concluding chapter, we present a summary of the contributions described in this work. We point out how the theoretical results can be applied to practical problems and how the theory can be developed in future work.

7.1 Conclusions

The contributions can be summarized as follows:

- **Modeling and Topology:** We defined a wide range of processes as a class of process networks. The framework allows the integration of subsystems modeled as nodes connected through flows among each other and through terminals to the environment. The subsystem’s state itself is described through its inventories and the internal dynamics are relevant only in that they have

to be dissipative. Due to the generality of the modeling framework, it applies to systems from different applications such as chemical plants, supply chains, reaction networks, convection and diffusion problems among many others. The main requirement is that balance equations for extensive quantities can be written and there exists a convex and uniquely defined potential. The latter property implies that the potential fields are smooth and the existence of a global potential can be replaced by the smoothness condition. In a thermodynamic system, these conditions follow directly from the first and second law of thermodynamics.

Algorithms define relations between extensive quantities (flows, inventories) and intensive quantities (potential gradients, potentials) which can be given either through physics in form of constitutive equations or through control and optimization algorithms. We introduce matrix algebra which allows to describe a process networks topology through tensors, matrices, and vectors. The compactness of the matrix modeling approach facilitates the use of network methods and theorems such as Tellegen's theorem improving compactness of proofs and theorems.

- **First Order Optimality and Duality:** We introduced the network content and cocontent as dual quantities. Process networks assume extremal points of the content and cocontent during evolution from an initial state to a final equilibrium point. This result is remarkable in its generality, since it does not need any assumption about the algorithm to define the flow. We showed that duality between extensive and intensive variables arises for the first order optimality conditions of process networks and are related to the topological duality of mesh versus nodal representations. For an explicit problem with given boundary conditions, the first order conditions assume optimality as a rigorous version of the minimum entropy production principle described by Prigogine [15] and Onsager [36, 37].

- **Second Order Optimality and Stability:** Stability of trajectories and convergence towards equilibrium points is based on the positivity of algorithms for flows and inventories. If natural algorithms, i.e., constitutive equations are positive, then trajectories and equilibria are stable.

These stability results follow directly from the convexity of the content and cocontent and the dissipativity of the flow connections. The content and cocontent can be used as a basis to derive a potential function which serves as a metric for the dissipation of the process network. The potential function then can be used to describe the process network as a gradient system. This point of view also allows to connect the stability results to classical Lyapunov stability theory.

- **Dynamics:** Variational principles exist for a wide range of partial differential equations such as for example diffusion or heat conduction equations. For our class of process systems, the first order time derivative is non-symmetric and hence, there does not exist a direct minimizer for the first order derivative. Under certain initial and boundary conditions, we can show a variational principle for the second order differential system of the process network. The results show that two driving forces dominate the evolution of the state of a process network along a trajectory. Firstly, there exists a driving force based on the entropy production of the system that drives the system to a state of minimum dissipation. Secondly, there is a driving force based on the inertia of the system that minimizes the change of the state. The two forces compete in a way that the inertial force tries to inhibit any changes while the dissipation seeks to change towards a state of minimum dissipation. We also show that there exists a feedback mechanism between the self regulation of flows in a process network and the inventories as states which can be related to the linear quadratic regulator or generally optimal control theory. Finally, we show that all process network flows and potentials seek the fastest way from the initial condition to a state of minimum entropy production where the Kirchhoff laws and constitutive equations can be seen as the natural boundaries limiting the rate at which the system can change.

- **Control and Optimization:** We demonstrated how control and optimization algorithms can replace or supplement the natural constitutive equations and thus alter the trajectory and equilibrium state of a process network. We showed that the natural objective of minimizing dissipation transforms into minimizing the difference between the actual state and the state desired

by the control system. We also show how process networks can be decomposed and highlight the connection between Lagrangean multipliers and the potentials at the nodes at which decomposition is performed.

- **Tellegen's Theorem as a Redundant Constraint:** We showed how the addition of a network theorem can strengthen the relaxation and hence improve solvability of a nonlinear dynamic optimization problem. We note an improvement in the gap between lower bound and upper bound as well as the number of nodes during the optimization process of this global optimization problem for a small scale example. This shows that if the system of differential equations is relaxed through convex approximations, the feasible region of the resulting relaxed NLP contains regions that violate topological properties of the flow network. The addition of Tellegen's theorem to the optimization problem thus functions as cuts to the feasible region reducing the size of the hypervolume of the relaxation.

- **Reservoir flow:** A reservoir modeling framework based on network theory has been developed. Network theorems have been used to prove stability and optimality properties for two-phase oil-water subsurface flow. The application of irreversible thermodynamics and a variational principle results in a gradient system description of the reservoir. For given pressure gradients, reservoir flow re-organizes itself to follow along the paths of least resistance and hence, maximize the fluid throughput for the reservoir. As a result, oil production is maximized if pressure gradients across the reservoir and particularly in the area about the water-oil front can be maximized.

  Displacement efficiency can be linked to thermodynamic principles and energy dissipation in the reservoir and oil recovery depends on how efficiently and selectively the energy generated by the injectors is used. We derive simple principles for the injection process that enforce maximum oil-water selectivity and minimum energy dissipation through control action at the wells which generally results into bang-bang type control for injectors and producers. We

propose a simple injection strategy based on the developed principle that does not require a detailed reservoir model and is based on simple feedback policies. The general principle of the proposed strategy is to maximize production flow subject to the amount of available energy from the injectors by generally minimizing loss of energy through control action and using the self-optimizing behavior of the reservoir. Once water breakthrough occurs, minimal control action is performed at the respective wells through simple on-off-strategies. The strategy can be effectively understood as adjusting the boundaries of the reservoir such that self-optimization leads to maximum production, and once water breakthrough occurs, the reservoir is periodically ”re-designed” at the boundaries, i.e. wells, and left for self-optimization until the next water breakthrough.

7.2 Future Work

There are several theoretical and practical directions in which this work can be extended. The most important aspects concern theoretical extensions towards multi-effect and multi-component systems, integration of common control algorithms (PID, MPC, RTO) for decentralized control, Tellegen's theorem as a redundant constraint in optimization for typical process system problems, and systematic evaluation of injection strategies based on rigorous optimization and realistic field cases.

- **Multicomponent Extension:** Future work can address the development of a framework for the integration of multiple extensive quantities into the topology of the network. Examples for reaction-diffusion or convection-diffusion systems should be developed in which several physical effects occur and several types of potentials cause flows on different time and length scales. The theoretical framework can be extended towards tensor descriptions. Inspiration can be drawn from Onsager's theory for the reciprocity about a local equilibrium using Onsager coefficients [36, 37].

- **Decentralized Optimization and Control Algorithms:** Actual control algorithms can be considered and tested for positivity such as PID controllers, model predictive control and real-time optimization. Stability and optimality conditions for combinations of different controllers on different time scales can be evaluated based on the convexity conditions for the potential function. Design of a control system for a process network example such as a petroleum platform or a small chemical plant based on the introduced concepts of relating the natural objective of a process to the economic objective and subsequent decomposition.

- **Observer Design:** Another possible application for the developed theory is the design of nonlinear observers for process networks based on the passivity condition and using Tellegen's theorem and a stability result from convergent systems theory [1]. The approach can be viewed as an adaptive control problem in which the model parameters are dynamically adjusted as soon as new information is available.

- **Tellegen's Theorem as a Redundant Contraint:** Tellegen's theorem can be tested in the context of different flow processes in global optimization. Any process that has a consistent definition of potentials and flows according to the Kirchhoff laws permits the decomposition into the basic network equations or, if not decomposable, Tellegen's theorem can be added as an additional constraint. Different versions of Tellegen's theorem can be used as a redundant constraint such as the integral or differential or a time-averaged version. Possibly, the integration of Tellegen's theorem into a relaxation strategy of a common global optimizer such as BARON could be of interest.

- **Reservoir Injection Optimization:** In order to compare different strategies for water injection of oil reservoirs, the dissipation based adaptive strategy developed in this work can be carried out using a rigorous algorithm and compared to optimization results based on optimal control algorithms. A useful reference would be to find simple reservoir case studies that can

be optimized to find the global optimum and used as a best case scenario to evaluate different strategies. As an interesting research direction, global optimization methods possibly combining the idea of Tellegen's theorem as a redundant constraint could be applied to simple reservoir studies and solved to global optimality as a benchmark case.

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Appendix A

Supply chains and the Second Law of Thermodynamics

A.1 Introduction

The theory developed in Chapter 3 can be applied to model financial, material and service flows in business systems, since conservation laws apply and the value of activities can be modeled using a convex potential. Decision making in a business system has to be understood as a multiobjective optimization problem [16, 56] on different time and hierarchical scales. Business organizations can be regarded as complex networks in which a combination of centralized and decentralized decision making aims to optimize a business' performance [49]. Regardless of the complexity, a business' objective to maximize its profit and as a consequence its total value is often implemented through very simple decentralized management policies that lead to self-optimizing structures using key indicators such as the Net Present Value or the Return on Investment [47]. We attempt to point out how this modeling approach can support understanding the network character of business systems, help explore self-optimizing structures, and develop optimization and control policies for complex and highly interconnected business systems [56].

A.1.1 Business Decision making and Finance

From a system point of view a business is governed by material, cash, service and information flow. We attempt to give a definition of a business that is adopted from [56].

Definition 21. *A business is a system encompassing financial relationships, material, service, and information flows. Business decision making is concerned with allocating resources in order to maximize the expected value of the business without incurring undue risk. The decisions can be grouped into the three distinct categories: (1) Investment, (2) Operation and (3) Finance.*

Essentially, a business is an integrated system of flows driven by management decisions in the areas of investment, operation and financing. Decisions have to be made at different hierarchical levels and timescales. The manager adjusts and controls the cash and material flows to maximize the profit objectives in every day operation. On the other hand, the financial analyst evaluates the performance of the company based on the companies financial statements by using key financial tools, i.e., she decides to invest according to the growth and financial situation of the company. In essence, the material, cash and service flows of a company are adjusted in a way to maximize the profit and as a consequence increase the total value or shareholder's/owners equity. From a system perspective, the various flows and processes in a company have to be controlled in a way to adjust the crucial parameters and achieve optimality both in terms of short term and long term investment.

To capture the dynamics of a business system, we can group the decisions into three different categories as depicted in Figure A.1:

1. Investment in fixed, variable and intangible assets.

2. Operation of systems and processes for production, service and technology development.

3. Financing of investment and operation through loans, stock issue and divestment.

The first category concerns how we manage the asset base, including purchase, maintenance, mergers and acquisitions, sale of fixed assets, intellectual property and current assets like cash and

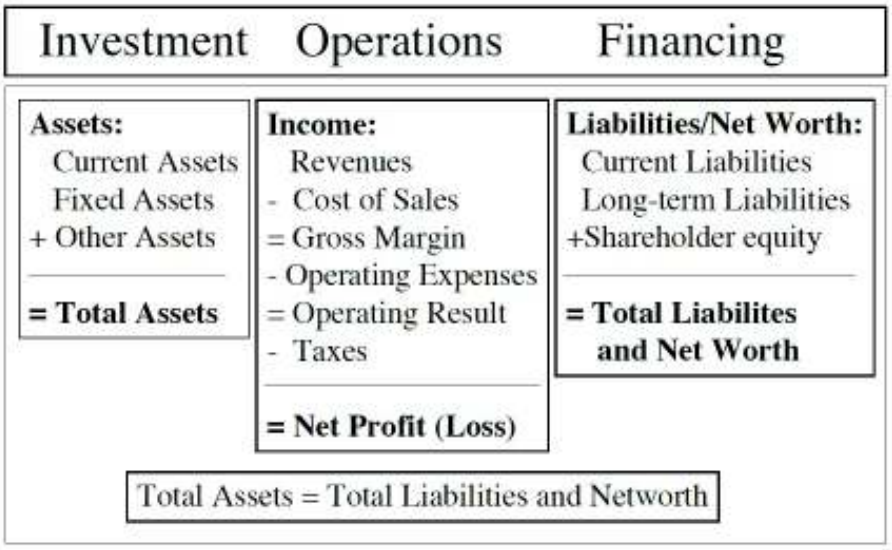

Figure A.1: A balance sheet (adapted from [19]) typically reports daily, weekly, monthly, quarterly or yearly results in the three categories as shown here. Each category is interlinked and together they give a complete picture of the financial state of the company. How the reporting is done is closely regulated by the Securities and Exchange Commission. However there are categories, like depreciation, that leave open possibilities for discretion.

inventory. The second category is concerned with the daily operation of the business, including sales, service, R&D, personnel, accounting and the flow of goods and services throughout the supply chain. The third category has to do with how the company integrates itself with the financial markets. In a further analysis, we can divide the decisions into short term and long term decisions. The short term decisions can be regarded as a continuous adjustment of parameters that is performed by a manager to maximize the profit. It concerns mainly the second category of operating decisions. Long term decisions are rather discrete and they have rather go/no go character. These decisions are mainly taken by a financial analyst who analyses the company and market structure based on the financial statement and determines potentials for growth and investment. She determines if a project is still profitable or a new project has sufficient market potential and makes discrete decisions about long term liabilities such as loans or purchasing fixed assets such as investment into new production facilities.

The flow behavior of assets such as inventories and cash into and out of the business system is

governed by conservation laws. Generally, the flow of assets can be modeled by developing a balance that conserves the assets.

In order to characterize the business system, we propose inventory balances for assets and liabilities. The assets can be sub-categorized into fixed assets, current assets and other assets.

$$a = \begin{cases} a^{current} - \text{ current assets (inventory and cash, accounts receivable)} \\ a^{fixed} - \text{ fixed assets (buildings equipment)} \\ a_{other} - \text{ other assets (patents, market position, licenses)} \end{cases}$$

and the liabilities into short term or current and long term liabilities

$$l = \begin{cases} l^{shortterm} - \text{ current liabilities (salaries, accruals, accounts payable, cost)} \\ l^{longterm} - \text{ financial instruments such as, mortgages, loans, etc} \end{cases}$$

For the assets the balance equations are given as

$$\frac{da_i}{dt} = F_{i,in}^{assets} - F_{i,out}^{assets} + p_i^{assets}, i = 1..N^{assets} \tag{A.1}$$

The different types of assets have to be treated independently, since their dynamic behavior differs, in particular in terms of the time scale. The current assets are modeled in a short time scale and changes can be regarded as continuous. The model equations for the current assets include all different kinds of assets that are connected to the final products, i.e. the assets that are finally sold to the costumers. This comprises raw material assets, intermediate and final products and cash related assets. We can further split the assets into the different categories that we have specified (current, fixed, and other) and

$$\frac{da_i^{current}}{dt} = F_{i,in}^{current} - F_{i,out}^{current} + p_i^{current}, i = 1..N^{current} \tag{A.2}$$

The current assets can be divided into two different kinds

$$\frac{da_i}{dt} = F_{i,in}^{inventory} - F_{i,out}^{inventory} + p_i^{inventory}, i = 1..N^{inventory} \tag{A.3}$$

and

$$\frac{da_i^{cash}}{dt} = F_{i,in}^{cash} - F_{i,out}^{cash} + p_i^{cash}, i = 1..N^{cash} \tag{A.4}$$

The balances for fixed and other assets are

$$\frac{da_i^{fixed}}{dt} = F_{i,in}^{fixed} - F_{i,out}^{fixed} + p_i^{fixed}, i = 1..N^{fixed} \tag{A.5}$$

$$\frac{da_i^{other}}{dt} = F_{i,in}^{other} - F_{i,out}^{other} + p_i^{other}, i = 1..N^{other} \tag{A.6}$$

The liabilities are modeled in a similar approach to the assets. There are current or short-term and fixed or long-term liabilities which have to be treated independently. The model equations for liabilities are given by

$$\frac{dl_i}{dt} = F_{i,in}^{liabilities} - F_{i,out}^{liabilities} + p_i^{liabilities}, i = 1..N^{liabilities} \tag{A.7}$$

which can be separated into

$$\frac{dl_i}{dt} = F_{i,in}^{shortterm} - F_{i,out}^{shortterm} + p_i^{shortterm}, i = 1..N^{shortterm} \tag{A.8}$$

$$\frac{dl_i}{dt} = F_{i,in}^{longterm} - F_{i,out}^{longterm} + p_i^{longterm}, i = 1..N^{longterm} \tag{A.9}$$

From a system point of view, the proposed set of equations that comprise the finance model of a company can be seen as a dynamic system. It consists of input-output variables i.e. the incoming and outgoing flows of assets and liabilities. The inventories of liabilities l_i and assets a_i define the state of a dynamical system of the following form uniquely

$$\frac{dv}{dt} = \phi(u,t) + p \tag{A.10}$$

In our finance model, we intend to propose consistent relationships for the regarded inventories in a general framework. In essence, the inventory balances are conservation laws so that the inventories in the modeling framework are conserved. From a process network perspective, the balance equations model the company as a node in which transformation and storage of inventories can occur as depicted in figure A.2. The input-output values such as the inventory and liability flows define the boundaries of the model that can provide connections to other nodes or they can be control variables to achieve a certain objective. The flows and production terms on the right hand side of the system of differential equations for the assets and liabilities that we have proposed are connected in many cases. For example, the inventory balances production terms are connected if a raw material A and B are transformed to a product C that is then sold on the market. Therefore, one has to find relationships that relate the transformation process to the constraints and properties of the business system. In general, production is limited to a certain capacity and therefore

$$0 \leq p_i \leq p_i^{limit} \tag{A.11}$$

The production rate in addition is related to the values of the different inventories that are involved in the production process. If raw materials A and B are purchased and converted into C with a higher value than the raw materials, then the production rate naturally depends on the values of prices of the raw materials and final product. A decrease of the market price of the product must have a negative

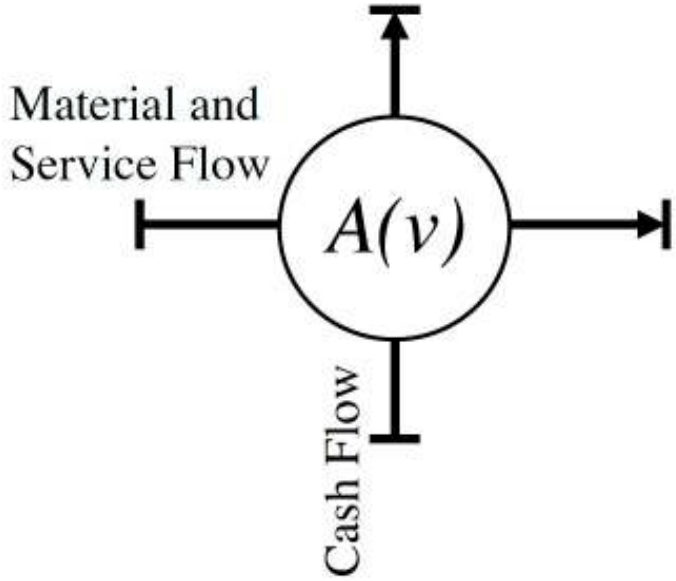

Figure A.2: In this paper we view the business as an input-output system. There are two flows of interest. The first concerns the flow of goods and services through the system. The second concerns the flow of cash. These flows must be managed so that the business objective(s), in this case denoted by $A(v)$, where v is the state of the system, is (are) maximized.

effect on production as well as an increase of the raw material prices and therefore costs force a decision to decrease the production rate. Specific laws for the production rate will be proposed in later sections.

The incoming and outgoing flows of inventory can be regarded as continuous and they are the connections to other business or customers. The magnitude of the flows is dependent on the profit that can be achieved by purchasing raw material and selling the final product for a certain price or value. The higher the price difference that can be achieved after withdrawing the effective cost for production, general operation of the business and transportation from the supplier to the costumer the higher the flow will be.

The cash flow and production term of the business depends on several aspects. The production term usually can only consume cash, since cash can only be generated through sales. Cash is consumed in a production process if for producing a certain product, it is necessary to invest a set of

raw materials and in addition cash assets for energy or labor etc that is consumed per product item. The incoming flows for cash are revenues from sales and cash that is generated through loans that are taken out. The revenues have a continuous character, since products can be assumed as continuously sold in a continuous flow. The incoming cash through contracting new loans is rather a discrete change that at the same time affects the long term liabilities. Similarly the outgoing cash flows are loans or long term liabilities that are paid off to reduce the amount of interest by decreasing the total debt. The continuous cost from purchasing raw materials, for salaries of employees, interest and income tax are effectively accounted for in the current liabilities.

Generally, the cash assets are treated as the current outstanding credit or effective cash on hand whereas the current liabilities are the debit. The current liabilities are generally due after a period of months to one year, where one flow item in between the short term liabilities and cash assets is modeled to compensate the otherwise growing balances for cash assets and short term liabilities. This can be modeled either as a continuous flow or by a discrete transfer dependent on the terms of accounts payable and accounts receivable.

To increase production capacities, production sites and equipment are purchased or built and employees are hired which in fact means a discrete increase in fixed assets and in turn a discrete increase in long term liabilities. If there is enough cash on hand, increasing fixed assets can also be financed through the short term liabilities or effectively the cash balance.

If relationships or functions are established for the flows and the production terms of the business system and the boundaries and initial conditions are given the system will develop over time into a certain state.

A.2 Value of Assets and Liabilities

In the last section, we have been balancing the assets and liabilities in terms of their quantities and derived conservation equations. In financial statements of businesses, the assets and liabilities are

balanced in terms of their total value. For our modeling approach, it is therefore necessary to assign a nominal value per unit w_i to each asset or liability so that the total value of assets and liabilities is given as a function of the inventories and their corresponding values

$$A(v) = \sum_{i}^{N^assets} I_i w_i = \mathbf{I^T w}, \text{value of all assets (bookvalue) [Value]} \tag{A.12}$$

$$L(v) = \sum_{i}^{N^assets} L_i w_i = \mathbf{L^T w}, \text{ liabilities [Value]} \tag{A.13}$$

$$\tag{A.14}$$

The total value of assets can be split into different categories

$$A = \underbrace{A^{\text{cash}} + A^{\text{inventory}}}_{\text{current assets}} + A^{\text{fixed}} + A^{\text{other}}$$

consisting of current assets, fixed assets, and other assets. In a similar approach, the total liabilities comprise

$$L = L^{\text{short-term}} + L^{\text{long-term}}$$

To determine the net worth or shareholder/owner equity, the total value of liabilities are subtracted from the total value of assets

$$E = A - L \tag{A.15}$$

The net worth E of a business is a key measure, since the ultimate goal for every business is to constantly increase the net worth on a long term basis. Decisions for investment, financing and operation have to be made such that shareholder equity increases possibly with the maximal possible rate within the constraints that are posed onto the regarded business system. After defining the value functions, we can balance the total value flows for the business which draws a connection to the

operating cash balance. The operations balance can be developed similarly to the asset and liabilities balance

$$\left\{ \frac{\text{accumulation of value}}{\text{time}} \right\} = \left\{ \text{net flow of value} \right\} + \left\{ \text{generation/destruction of value} \right\}$$

Here, we intend to determine the relations between the incoming and the outgoing values and the generation term for value. The time derivative of the shareholder equity is used as a starting point

$$\frac{dE}{dt} = \frac{dA}{dt} - \frac{dL}{dt} \tag{A.16}$$

An increase in the total asset value ($\frac{dA}{dt}$) leads to an increase in the net value of the business as well as a decrease in the total liabilities leads to an increase in the net value. The value balance for each asset $A_i$is

$$\frac{dA_i}{dt} = (F_{i,in} - F_{i,out}) w_i^{asset} + w_i^{asset} p_i, i = 1..N^{assets} \tag{A.17}$$

analogous for the liabilities

$$\frac{dL_i}{dt} = (F_{i,in}^{liabilities} - F_{i,out}^{liabilities}) w_i^{liabilities} + w_i^{liabilities} p_i^{liabilities}, i = 1..N^{liabilities} \tag{A.18}$$

If we want the total change of asset and liability values we will have to sum up the equations for the individual assets A.17 and liabilities A.19

$$\frac{dA}{dt} = \sum_{i=1}^{N^{assets}} (F_{i,in} - F_{i,out}) w_i^{asset} \tag{A.19}$$

The production terms cancel out for the sum of the assets in equation A.19, since conservation laws

also hold for the production terms. For every set of asset (raw materials and cash) that is converted to final or intermediate products the values are conserved. For example, raw material A_1 and A_2 are converted into final product A_4. If we produce a single item of the final product, the product value consists of the raw material values. In fact, the true value of a product also has to include the costs that occur in operation of the business. Since the cost of operation is not explicitly associated with a single product but with the entire set of products that are produced in a business, we chose to include cost of operation as a general asset independent term in the short term liabilities. For the liabilities, we have

$$\frac{dL}{dt} = \sum_{i=1}^{N^{liabilities}} (F_{i,in}^{liabilities} - F_{i,out}^{liabilities}) w_i^{liabilities} + \sum_{i=1}^{N^{prodterms}} w_i^{liabilities} p_i^{liabilities} \tag{A.20}$$

The total change of assets $\frac{dA}{dt}$ can be split up into two equations for the change in cash asset values $\frac{dA^{cash}}{dt}$ and the change in inventory.

$$\frac{dA^{cash}}{dt} = \sum_{i=1}^{N^{cash}} (F_{i,in}^{cash} - F_{i,out}^{cash}) w_i^{cash} + p_i^{cash} w_i^{cash} \tag{A.21}$$

$$\frac{dA^{inv}}{dt} = \sum_{i=1}^{N^{inv}} (F_{i,in}^{inv} - F_{i,out}^{inv}) w_i^{inv} + p_i^{inv} w_i^{inv} \tag{A.22}$$

The value change of the assets $\frac{dA}{dt}$ and liabilities $\frac{dL}{dt}$ over time can be split up in its components.

$$\frac{dE}{dt} = \frac{dA^{inventory}}{dt} \frac{dA^{cash}}{dt} + \frac{dA^{fixed}}{dt} + \frac{dA^{other}}{dt} - \frac{dL^{shortterm}}{dt} - \frac{dL^{longterm}}{dt} \tag{A.23}$$

To further unravel the relationship that lead to creation of value in a company, we have to divide the value change of assets into investment/finance and operational changes. $\frac{dA^{inventory}}{dt}$ is clearly of operational nature and connected to every day transfer of assets that are connected to sales and operational value creation. The changes in the value of fixed assets $\frac{dA^{fixed}}{dt}$ other assets $\frac{dA^{other}}{dt}$ and the long term

liabilities $\frac{dL^{longterm}}{dt}$ are clearly connected to investment and finance decisions. The other terms on the right hand side of equation A.23 have a hybrid character; they contain both terms that are connected to continuous operation and discrete finance and investment terms. The right hand side can be further decomposed into operation and finance variables

$$\begin{aligned}\frac{dE}{dt} = \frac{dA^{inv}}{dt}\frac{dA^{cash,op}}{dt} + \frac{dA^{cash,fin}}{dt} + \frac{dA^{fixed}}{dt} + \frac{dA^{other}}{dt} \\ - \frac{dL^{shortterm,op}}{dt} - \frac{dL^{shortterm,fin}}{dt} - \frac{dL^{longterm}}{dt}\end{aligned} \tag{A.24}$$

The investment and finance related terms do not create any value, since they are connected in the following way

$$0 = \frac{dA^{cash,fin}}{dt} + \frac{dA^{fixed}}{dt} + \frac{dA^{other}}{dt} - \frac{dL^{shortterm,fin}}{dt} - \frac{dL^{longterm}}{dt} \tag{A.25}$$

This is due to the fact that for example an acquisition of fixed assets creates the same amount of obligations on the liabilities side. Purchasing fixed assets requires either to charge the obligations connected to the fixed assets to the short term liabilities or it requires a new loan or mortgage on the purchased fixed asset. If the total balance of cash assets and short term liabilities is on credit side, it can be possible to finance the acquisition of the fixed asset(s) directly through current items, but for large investment, it is always necessary to finance through long term liabilities. Using relation A.25, the finance and investment terms cancel out and equation A.24 simplifies to

$$\frac{dE}{dt} = \frac{dA^{inv}}{dt} + \frac{dA^{cash,op}}{dt} - \frac{dL^{shortterm,op}}{dt} \tag{A.26}$$

In a business system, although asset flows and operation persistently change, steady state flows for the inventory and operations are desired dependent on how market fluctuations allow. Supply and demand behavior play a crucial role and constantly change on global markets and require constant

adjustment of material in stock. Nevertheless, assuming that the business system and the market show a steady state behavior on a long term consideration, we can for now assume that the inventory is constant and does not effectively effect the value creation $\frac{dE}{dt}$.

$$\frac{dE}{dt} = \frac{dP}{dt} = \frac{dA^{cash,op}}{dt} - \frac{dL^{shortterm,op}}{dt} \tag{A.27}$$

In financial terms, equation (A.27) shows the change of profit of a company. The profit over a certain period of time plays a key role in creating value. If the owner's equity is supposed to be maximized over a certain period of time, it follows that the change of profit has to be maximized to achieve this goal. To further explain the components of the profit change balance, equation A.27, we have to introduce several new terms and show the detailed terms that the cash asset change and short term liability change consist of.

The effective income $\frac{dA^{cash,op}}{dt}$ of a company are accounts payable from sales of products, the so called revenues R

$$R = \sum_{i=1}^{N^{products}} F_{i,out}^{products} w_{i,out}^{products} \tag{A.28}$$

where $w_{i,out}^{products}$ is the selling price. The effective debt that is charged to the short term operational liabilities $\frac{dL^{shortterm,op}}{dt}$ can be regarded as cost or in financial terms cost of sales and consists of the following terms

$$C = C_{rawmaterials}(F) + C_{depreciation}(a^{fixed}) + C_{operation} + C_{incometax}(P) + C_{transaction}(F) + C_{interest} \tag{A.29}$$

where $C_{rawmaterials}(F) = \sum_{i=1}^{N^{rawmat}} F_{i,in} w_{i,in}^{rawmat}$.

The cost consists of different items namely raw material cost, cost for depreciation, cost of operation including R&D, administrative cost, energy and utilities and salaries for employees, tax on income and cost for transportation of inventory from the supplier and to the costumer, transaction

costs for financial money transfers, and cost due to interest from long term debt. The profit change is given as

$$\frac{dP}{dt} = R - C = \phi_P \tag{A.30}$$

If the equations is integrated over the reporting period T, we obtain

$$P = \int_t^{t+T} \phi_P ds \tag{A.31}$$

To further point out the crucial criteria for an enterprise to make profit, we substitute equation A.28, A.22, and A.21 into equation A.30.

$$\begin{aligned}\frac{dP}{dt} = &\sum_{i=1}^{N^{assets}} F_{i,in}^{asset} w_i^{asset} - \sum_{i=1}^{N^{assets}} F_{i,out}^{asset} w_i^{asset} + \sum_{i=1}^{N^{products}} + F_{i,out}^{products} w_{i,out}^{products} - \sum_{i=1}^{N^{rawmat}} F_{i,in}^{rawmat} w_{i,in}^{rawmat} \\ &- (C_{depreciation}(a^{fixed}) + C_{operation} + C_{incometax}(P) + C_{transaction}(F)) + C_{interest}\end{aligned} \tag{A.32}$$

Here, we have the following relationships for the flows

$$F_{i,in}^{asset} = F_{i,in}^{rawmat} F_{i,out}^{asset} = F_{i,out}^{products} \tag{A.33}$$

This leads to the following equations for the the change of profit balance

$$\begin{aligned}\frac{dP}{dt} = &\sum_{i=1}^{N^{products}} F_{i,out}^{products} (w_{i,out}^{products} - w_i^{asset}) - \sum_{i=1}^{N^{assets}} F_{i,in}^{rawmat} (w_i^{asset} - w_i^{rawmat}) - \sum_{i=1}^{N^{rawmat}} F_{i,in}^{rawmat} w_{i,in}^{rawmat} \\ &- (C_{depreciation}(a^{fixed}) + C_{operation} + C_{incometax}(P) + C_{transaction}(F)) + C_{interest}\end{aligned} \tag{A.34}$$

In order to make profit, i.e. to achieve that the change of profit $\frac{dP}{dt}$ is positive, the cost items in equation A.34 have to be covered by the markup that is realized through selling the products. The margin has

to cover the cost of operation, the loss of value through appreciation of fixed assets, the interest on the long term liabilities the transaction costs on cash and transportation costs of inventory, and the cost of operation such as R&D expenses, administrative costs and wages for employees. It also has to cover the cost that occurs if assets are purchased for a higher price than their actual value from the suppliers. We can regard the process from purchasing raw materials, transporting, conversion to products, and sales and transportation to the costumer as a branch of a value added network. Every transaction or activity adds value to the the asset and increases its price. We will suggest a framework in the following sections that takes these ideas into account and describes the business as as a value added network.

As can be seen, value in a company can only be created if the operations create a positive change of profit. This is highly dependent on the interconnections of the business with suppliers and costumers, i.e. the market. The market imposes constraints on the business; costumers have a certain demand which is dependent on the price of the products they purchase. The price is highly dependent on demand and supply and the business has to offer a price to the customer that allows to the business excel competitors. The competitiveness therefore is strongly connected to the business' ability to minimize the cost and keep the selling price of product as low as possible. We will address the optimization problem that has to be solved in the following sections.

A.3 The Enterprise as a Value Added Chain

In the previous section, we modeled the processes in a business system as a set of differential equations that describe the dynamic behavior of assets and liabilities of a business. We regarded the business systems as an independent entity that intends to maximize its profit under the constraints imposed by the environment. Figure A.3 shows the finance model of a business as a single node that is connected to the suppliers through branches from the terminals to the node on the right hand side and branches from the node to the customer terminals. We can see different activities about the node

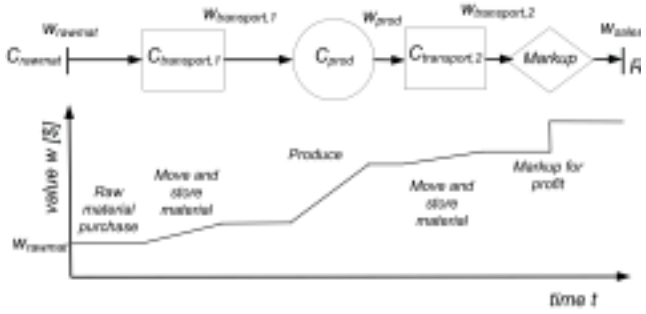

Figure A.3: The value chain tracks how process operations add value to goods as they move through the production system. The last section includes the price markup as a value added step.

that have an effect on the value of the assets flowing through the business system. Raw material or intermediate products are purchased for a certain price $w_{rawmat,i}$ at the supplier terminal and transported to the business for production. The value of the incoming assets increase according to the cost of transportation on their way to the production and storage facility. After transforming services raw material and intermediate products to final products the products are shipped to the costumer. The production process further increases the value of the products in the transformation process. The product value represents at least the values of raw materials that it consists of. It also includes labor, utilities, energy and service that is invested to produce the final product. Subsequently, the final products are sold on the market. For the yet to determine selling price, there are different scenarios that finally lead to the selling price. Obviously, the products could be sold for the price of their internal value. This is in particularly done if the customer is part of the same supply network, i.e. the business system and the costumer belong to the same company. The product is therefore sold at cost and the selling price can be regarded as a transfer price from one part of the company to the next. Generally, the product is sold for a higher price as the nominal value. The upper limit of the selling price is commonly determined by the costumer or market, since the business unit has to ensure that it stays competitive compared to other businesses. The value that can be created through a higher selling price leads to a markup and is booked as profit in the operations balance of the business unit. Each business unit contributes to the total profit of a company and its total competitiveness is determined

by the overall performance on the market. In order to achieve this objective, the entire company consisting of all business units has to adjust its pricing policies in a way that they are optimal when interacting with the market through sales of products. The structure of decision making can be seen as depicted in figure A.4. To embed the enterprise into the market or an economic structure, the flows of

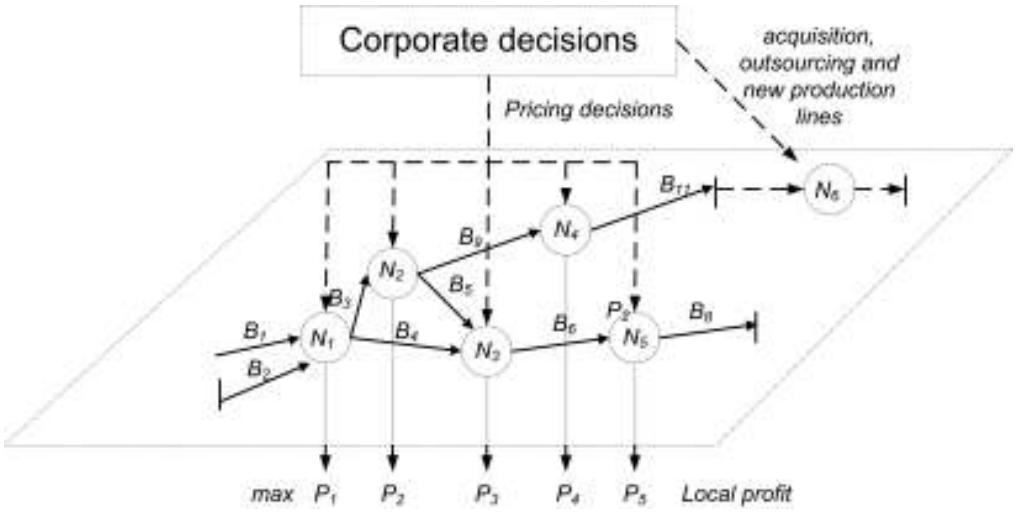

Figure A.4: A company can be seen as a complex structure in which independent business units are interconnected through asset and liability flows. The decision making process can be grouped into decentralized decisions that are executed by the individual units and centralized decisions such as pricing of products, mergers, acquisitions and new production lines.

the business system are connected to other independent business systems through the flows of inventories and liabilities. In many cases, companies are a complex network of independent entities that are managed in a decentralized fashion. As a consequence, the independent business units in a company are connected and coupled but they are managed and optimized regarding their value independently. An enterprise consists of many independent business units. As an example we can consider a supply network, where products are produced in a factory and then shipped to a warehouse, distribution center and finally to the retailer where they are purchased by the costumer. Each of these business units individually tries to maximize profit and is coupled to the upstream and downstream units through flow of products and cash transactions. An enterprise can be pictured as shown in figure A.5 with

connections of flows between different units and terminals that depict connections to the market be it suppliers on the left hand side or customers on the right hand side. Inside the business network, complex structures can be lumped together to reduce complexity and be described as a single node. As explained in the previous section, we assign values to the inventories, cash assets, and liabilities.

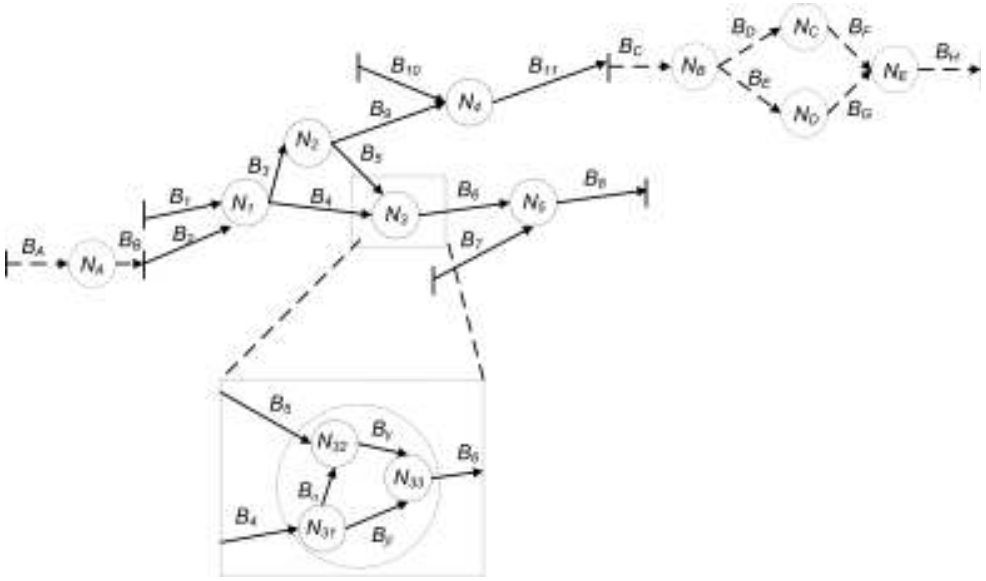

Figure A.5: The activity network has a hierarchical structure. Products from one activity form the resources for another. Activities can be lumped together. The terminals are connected to external markets or other networks. At these junctions the resource and sales costs are defined.

We assign values according to the activities that are performed on assets and liabilities to account for internal cost that is connected to each activity. Figure A.5 shows how the flows of manufactured goods flow through a network of activities. Activities can be combined and lumped in complex manners, not unlike an electrical circuit. The behavior of each activity and its financial performance is described by the conservation laws for assets and liabilities that were previously introduced.

Appendix B

Derivation of Tellegen's Theorem

The derivation of Tellegen's Theorem in this section is based on the one found in [24]. It shows an extension to process networks including chemical production. An illustrative and fairly general example is also provided alongside the derivation.

First, let $Z = Z(t)$ be a variable denoting the inventory of a process usually being extensive quantities (internal energy, mass, electric charge, etc.). The general conservation law for a process can be written

$$\dot{Z} = p(Z) + \sum_{i=i}^{m} f_i \tag{B.1}$$

where $p(Z)$ represents generation of the inventory Z (e.g. due to a chemical reaction) and f_i represents all $m,\ m \geq 0$, flows of the same inventory in and out of the process. The time dependence of Z will in most equations not be stated explicitly.

Now consider a process network, i.e., a network in which each vertex is a process, with n_p processes and n_t terminals. Assume that the processes are numbered 1 to n_p and that the terminals are

numbered $n_p + 1$ to $n_p + n_t$. Denote the flow from from vertex i to vertex j by f_{ij}, and note that

$$f_{ij} = -f_{ji} \tag{B.2a}$$

$$f_{jj} = 0 \tag{B.2b}$$

Equation (B.2b) states that there are no flows from a node to itself. Each node j has an associated potential $w_j = w_j(t)$, e.g. pressure or voltage, where the time dependence of the potential will be assumed implicitly. The potential is commonly relative to the potential at the 0-node, as voltage often is measured relative to ground, or pressure measured relative to atmospheric pressure. The potential of the 0-node is assumed to be zero (cf. ground).

An example of such a network is shown in Figure B.1. Note that the processes are numbered $1-4$ and that the terminals (integrating the network with the environment) are numbered $5-6$. The 0-node is implicitly present in the figure, and represents the environment. For this process network, the number of processes is $n_p = 4$, the number of terminals is $n_t = 2$, and the number of nodes is $n_p + n_t = 6$.es is $n_p + n_t = 6$. For processes in a network, a more convenient form of the conservation

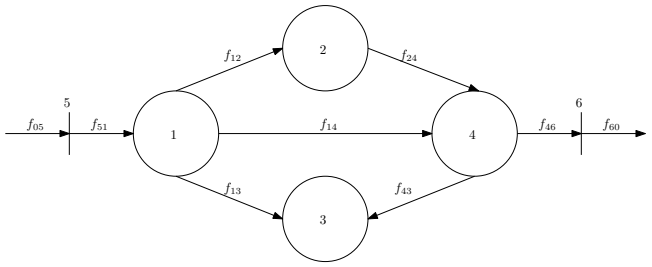

Figure B.1: A fairly general example of a process network.

law (B.1) is

$$\dot{Z}_j = p_j + \sum_{i=0}^{n_p+n_t} f_{ij}, \quad j = 0, 1, 2, \ldots, n_p + n_t \tag{B.3}$$

where (B.2b) is assumed. To illustrate the conservation law for processes in a process network, it is applied to two of the nodes in Figure B.1. As a first example, consider node 2, which is a process.

Equation (B.3) gives

$$\dot{Z}_2 = p_2 + f_{02} + f_{12} + f_{22} + f_{32} + f_{42} + f_{52} + f_{62} \tag{B.4}$$

Recognizing that that the majority of the flows are zero, $f_{02} = f_{22} = f_{32} = f_{52} = f_{62} = 0$, and that $f_{42} = -f_{24}$ (cf. equation (B.2a)), equation (B.4) reduces to

$$\dot{Z}_2 = p_2 + f_{12} - f_{42} \tag{B.5}$$

which can be seen directly from Figure B.1. As a second example, consider node 5, which is a terminal. Again using equation (B.3),

$$\dot{Z}_5 = p_5 + f_{05} + f_{15} + f_{25} + f_{35} + f_{45} + f_{55} + f_{65} \tag{B.6}$$

Also here the majority of flows are zero, $f_{25} = f_{35} = f_{45} = f_{55} = f_{65} = 0$, and $f_{15} = -f_{51}$. For a terminal, there is neither accumulation ($\dot{Z}_5 = 0$) nor production ($p_5 = 0$), so equation (B.6) reduces to

$$f_{51} = f_{05} \tag{B.7}$$

This can again be verified by inspecting Figure B.1.

For the derivation of Tellegen's Theorem, consider two process networks with the same topology and (possibly) different operating conditions (i.e., states). For the remainder of this derivation, this will be thought of as the same network at two (possibly) different time instants t_1 and t_2. First, consider equation (B.3) at time instant t_1,

$$\dot{Z}_j(t_1) = p_j(t_1) + \sum_{i=0}^{n_p+n_t} f_{ij}(t_1), \quad j = 0, 1, 2, \ldots, n_p + n_t \tag{B.8}$$

Then, multiply by the potential of some node j at t_2, $w_j(t_2)$, to get

$$w_j(t_2)\dot{Z}_j(t_1) = w_j(t_2)p_j(t_1) + w_j(t_2)\sum_{i=0}^{n_p+n_t} f_{ij}(t_1), \quad j = 0,\ldots,n_p+n_t \tag{B.9}$$

Note that the summation is taken over i, so that the potential in the last term can be placed inside the summation,

$$w_j(t_2)\dot{Z}_j(t_1) = w_j(t_2)p_j(t_1) + \sum_{i=0}^{n_p+n_t} w_j(t_2)f_{ij}(t_1), \quad j = 0,\ldots,n_p+n_t \tag{B.10}$$

Then, taking the sum over all nodes, i.e., all processes, terminals and the 0-node, gives

$$\sum_{j=0}^{n_p+n_t} w_j(t_2)\dot{Z}_j(t_1) = \sum_{j=0}^{n_p+n_t} w_j(t_2)p_j(t_1) + \sum_{j=0}^{n_p+n_t}\sum_{i=0}^{n_p+n_t} w_j(t_2)f_{ij}(t_1) \tag{B.11}$$

For terminals, there is neither accumulation ($\dot{Z} = 0$) nor production ($p = 0$), so the sum will not be taken over terminals in the two leftmost terms. Hence, equation (B.11) reduces to

$$\sum_{j=0}^{n_p} w_j(t_2)\dot{Z}_j(t_1) = \sum_{j=0}^{n_p} w_j(t_2)p_j(t_1) + \sum_{j=0}^{n_p+n_t}\sum_{i=0}^{n_p+n_t} w_j(t_2)f_{ij}(t_1) \tag{B.12}$$

As the potential of the 0-node is assumed to be zero, $w_0(t) = 0\ \forall\ t$, all summations over j start at 1 instead of 0,

$$\sum_{j=1}^{n_p} w_j(t_2)\dot{Z}_j(t_1) = \sum_{j=1}^{n_p} w_j(t_2)p_j(t_1) + \sum_{j=1}^{n_p+n_t}\sum_{i=0}^{n_p+n_t} w_j(t_2)f_{ij}(t_1) \tag{B.13}$$

For clarity in the last step of the derivation, consider the last term and expand the inner sum from $i = 1$ to $i = n_p + n_t$, treating the flows to and from the environment ($i = 0$) separately,

$$S \equiv \sum_{j=1}^{n_p+n_t}\sum_{i=1}^{n_p+n_t} w_j(t_2)f_{ij}(t_1) = \sum_{j=1}^{n_p+n_t} w_j(f_{1j} + f_{2j} + f_{3j} + \cdots + f_{nj}) \tag{B.14}$$

where S is just shorthand notation for the double sum, and $n = n_p + n_t$. Expanding the remaining sum gives

$$\begin{aligned} S = & w_1(f_{11} + f_{21} + f_{31} + \cdots + f_{n1}) \\ & + w_2(f_{12} + f_{22} + f_{32} + \cdots + f_{n2}) \\ & + w_3(f_{13} + f_{23} + f_{33} + \cdots + f_{n3}) \\ & + \cdots \\ & + w_n(f_{1n} + f_{2n} + f_{3n} + \cdots + f_{nn}) \end{aligned} \tag{B.15}$$

For reasons that will become apparent below, equation (B.2b) is applied to all flows "above the diagonal", i.e., for the flows f_{ij} where $i > j$, to get

$$\begin{aligned} S = & + w_1 f_{11} - w_1 f_{12} - w_1 f_{13} - \cdots - w_1 f_{1n} \\ & + w_2 f_{12} + w_2 f_{22} - w_2 f_{23} - \cdots - w_2 f_{2n} \\ & + w_3 f_{13} + w_3 f_{23} + w_3 f_{33} - \cdots - w_3 f_{3n} \\ & + \cdots \\ & + w_n f_{1n} + w_n f_{2n} + w_n f_{3n} + \cdots + w_n f_{nn} \end{aligned} \tag{B.16}$$

From equation (B.2b), the flows "on the diagonal" are zero, and hence

$$\begin{aligned} S = & - w_1 f_{12} - w_1 f_{13} - \cdots - w_1 f_{1n} \\ & + w_2 f_{12} - w_2 f_{23} - \cdots - w_2 f_{2n} \\ & + w_3 f_{13} + w_3 f_{23} - \cdots - w_3 f_{3n} \\ & + \cdots \\ & + w_n f_{1n} + w_n f_{2n} + w_n f_{3n} + \cdots \end{aligned} \tag{B.17}$$

Collecting the potentials associated with the same flow results in

$$\begin{aligned} S = &- f_{12}(w_1 - w_2) - f_{13}(w_1 - w_3) + \cdots - f_{1n}(w_1 - w_n) \\ &- f_{23}(w_2 - w_3) - \cdots - f_{2n}(w_2 - w_n) \\ &- \cdots - f_{3n}(w_3 - w_n) - \cdots \end{aligned} \tag{B.18}$$

Defining $\Delta w_{ij}(t) = w_i(t) - w_j(t)$ allows S to be written as

$$\begin{aligned} S = &- f_{12}\Delta w_{12} - f_{13}\Delta w_{13} + \cdots - f_{1n}\Delta w_{1n} \\ &- f_{23}\Delta w_{23} - \cdots - f_{2n}\Delta w_{2n} \\ &- \cdots - f_{3n}\Delta w_{3n} - \cdots \end{aligned} \tag{B.19}$$

Note that equations (B.15) - (B.19) lend themselves to matrix/vector notation. This can be useful to have in mind when reading derivations of Tellegen's Theorem with matrices.

Defining a flow f_{ij} to be positive if $i < j$, then a flow will be positive over a pressure drop Δw_{ij}, $i < j$, which is a sign convention that makes physical sense[1]. Defining n_f to be the number of positive flows in the process network (this does not exclude any flows), and a summation variable k that runs over all the positive flows, the double sum (including the $i = 0$ term) can be written

$$\sum_{j=1}^{n_p+n_t} \sum_{i=0}^{n_p+n_t} w_j(t_2) f_{ij}(t_1) = -\sum_{k=1}^{n_f} \Delta w_k(t_2) f_k(t_1) + \sum_{j=1}^{n_p+n_t} w_j(t_2) f_{0j}(t_1) \tag{B.20}$$

The last sum goes over flows from the environment (the 0-node with $i = 0$). There are no flows between the environment and processes, all flows connecting the process network to the environment

[1] Note that this sign convention is nothing more than that - a sign convention. It does not restrict the physical direction of flows, only which sign to put on a flow in a given direction. Notice that the arrows in Figure B.1 does not follow this convention.

are connected to terminals. Hence, the last sum can go from $j = n_p + 1$ to $j = n_p + n_t$,

$$\sum_{j=1}^{n_p+n_t} \sum_{i=0}^{n_p+n_t} w_j(t_2) f_{ij}(t_1) = -\sum_{k=1}^{n_f} \Delta w_k(t_2) f_k(t_1) + \sum_{j=n_p+1}^{n_p+n_t} w_j(t_2) f_{0j}(t_1) \tag{B.21}$$

Substituting this into equation (B.13) leads to

$$\sum_{j=1}^{n_p} w_j(t_2) \dot{Z}_j(t_1) = \sum_{j=1}^{n_p} w_j(t_2) p_j(t_1) + \sum_{j=n_p+1}^{n_p+n_t} w_j(t_2) f_{0j}(t_1) - \sum_{k=1}^{n_f} \Delta w_k(t_2) f_k(t_1) \tag{B.22}$$

Equation (B.22) is a fairly general formulation of Tellegen's Theorem. However, the equation also holds for variables transformed by network operators, e.g. linear filters, Fourier transforms, and time averaging [42].

Appendix C

Optimality and Stability: Theory

C.1 Lyapunov Stability

Starting with

$$V(\bar{\mathbf{Z}}) = \int_0^{\bar{\mathbf{W}}(\bar{\mathbf{Z}})} \bar{\mathbf{F}}(\bar{\mathbf{Z}}) d\bar{\mathbf{W}}(\bar{\mathbf{Z}}) \tag{C.1}$$

we use the resistive constitutive equations

$$V(\bar{\mathbf{Z}}) = \frac{1}{2}\bar{\mathbf{W}}(\bar{\mathbf{Z}})^T \mathbf{K}\bar{\mathbf{W}}(\bar{\mathbf{Z}}) \tag{C.2}$$

Kirchhoff voltage law and the capacitive constitutive equations

$$V(\bar{\mathbf{Z}}) = \frac{1}{2}\bar{\mathbf{Z}}^T \Phi \bar{\mathbf{Z}} \tag{C.3}$$

where $\Phi = \mathbf{C}^{-1}\mathbf{A_R}\mathbf{K}\mathbf{A_R}^T\mathbf{C}$. It follows that $V(\bar{\mathbf{Z}}) \geq 0$ for all $\bar{\mathbf{Z}}$ and it has to be shown that

$$\frac{dV(\bar{\mathbf{Z}})}{dt} = \frac{1}{2}\bar{\mathbf{Z}}^T \Phi \frac{\bar{\mathbf{Z}}}{dt} < 0 \tag{C.4}$$

From the co-content formulation, we can derive that

$$\frac{dV}{dt} = \mathbf{F_R}^T \frac{d\mathbf{W_R}}{dt} \tag{C.5}$$

using Tellegen's theorem in the deviation variables

$$\mathbf{F_R}^T \frac{\bar{\mathbf{W}}_\mathbf{R}}{dt} = -\frac{d\bar{\mathbf{Z}}}{dt}^T \frac{\bar{\mathbf{w}}}{dt} \tag{C.6}$$

including the capacitive constitutive equations, we have

$$\frac{dV}{dt} = -\frac{\mathbf{d}\bar{\mathbf{Z}}}{dt}^T \mathbf{C}^{-1} \frac{d\bar{\mathbf{Z}}}{dt} \tag{C.7}$$

Since the constitutive equations are linear and positive, $\mathbf{C}^{-1}$ is a diagonal positive definite matrix and hence $\frac{dV}{dt} < 0$ for all $\bar{\mathbf{Z}}$.

C.2 Kirchhoff Voltage Law as Inequality Constraint

The dual formulation of the optimization problem of (3.215) is given as

$$\min_{\mathbf{F}} \quad G^{=} \int_0^T \left(\sum_{i=1}^{b} \int^{F_i} W_i dF_i \right) dt \tag{C.8}$$

$$s.t. \qquad \mathbf{F} = \mathbf{M^T f} \tag{C.9}$$

$$|\mathbf{MW}| \geq \mathbf{0} \tag{C.10}$$

$$\mathbf{F_R} = \mathbf{KW_R} \tag{C.11}$$

$$\mathbf{Z} = \mathbf{Cw} \tag{C.12}$$

$$\mathbf{Z}(0) = \mathbf{Z_0} \tag{C.13}$$

$$\mathbf{F_T} = \text{const} \tag{C.14}$$

where Kirchhoff's voltage law (C.10) is written as an inequality constraint.

Appendix D

Decentralized Control

D.1 Derivation of Linear Control Algorithm

The derivation of the linear control algorithm in Section 4.1 is given as follows. Starting with the general Kirchhoff current law

$$\mathbf{AF} = \mathbf{0} \tag{D.1}$$

we can decompose into

$$\frac{d\mathbf{Z}}{dt} + \mathbf{A_K F_K} + \mathbf{A_R F_R} = \mathbf{0} \tag{D.2}$$

$$\mathbf{F_T} + \mathbf{A_{K,T} F_K} + \mathbf{A_{R,T} F_R} = \mathbf{0} \tag{D.3}$$

replacing $\frac{d\mathbf{Z}}{dt} = \Phi(\mathbf{Z})$ and the control law follows.

Appendix E

Subsurface Flow

E.1 Undirected Incidence Matrix

Definition 22. *The $n_p \times n_f$ matrix $\mathbf{B_a}$ is called undirected connection matrix for the matrix elements b_{ij} being*

$$b_{ij} = \begin{cases} 1, & \textit{if flow } j \textit{ is connected with gridblock } i \\ 0, & \textit{if flow } j \textit{ is not connected with gridblock } i \end{cases}$$

One node of the network is set as reference or datum node P_0. The $(n_t - 1) \times n_f$ matrix $\mathbf{B}$, where the row that contains the elements B_{0j} of the reference node P_0 is eliminated, is called reduced undirected connection matrix.

E.2 Derivation of Reservoir Entropy

The second important network property is the uniqueness condition (Kirchhoff voltage law) for the complete reservoir. For the definition of the potentials we derive the entropy for a weakly compress-

ible fluid or solid. The entropy contributions for water, oil, and porous rock are given as

$$\mathcal{S}^{o,w,r} = Nk\left[\ln\left(\frac{V^{\alpha U^{c_v}}}{N^{\alpha+c_v}}\right) - \beta\frac{V}{N}\right] \tag{E.1}$$

where k is Boltzmann's constant and c_v is the specific heat capacity at constant volume, α is the thermal expansion, and β is the compressibility. We re-unite the different contributions for the entropy in (E.1)

$$\mathcal{S} = Nk\alpha\ln V + Nkc_v lnU - \beta V + \ln\left(\frac{1}{N}\right)^{\alpha+c_p} \tag{E.2}$$

$\mathcal{S}$ is concave and homogeneous degree one. The intensive variables and constitutive relations are now derived

$$\frac{\partial\mathcal{S}}{\partial V} = c_v k\frac{N}{U} = \frac{1}{T} \tag{E.3}$$

per definition, hence

$$U = c_v kNT \tag{E.4}$$

according to the principles of equipartition of the energy in statistical mechanics. We also see that $\frac{\partial U}{\partial T} = Nc_v \approx Nc_p$ for liquids.

$$\frac{\partial S}{\partial V} = Nk\alpha\frac{1}{V} - \beta = \frac{p}{T} \tag{E.5}$$

per definition, hence

$$(p/T) = -\beta + k\alpha\rho \tag{E.6}$$

, where $\rho = N/V$

$$Z = \frac{pV}{NRT} = \alpha - \beta\hat{V} + \gamma\frac{1}{\hat{V}} \tag{E.7}$$

where $\hat{V} = 1/\rho$. For liquids, we have $\gamma = 0$ while $\beta = 0$ for gases and generally $\alpha = 1$. From (E.6) we get

$$\rho = \frac{1}{\alpha}\left(\beta + \frac{p}{T}\right) = \frac{\beta}{\alpha} + \frac{1}{\alpha}\left(\frac{p}{T}\right) \tag{E.8}$$

and

$$\rho^{o,w,r} = \rho_0^{o,w,r} + c^{o,w,r}(p - p_0) \tag{E.9}$$

with $c = 1/\alpha T$ and

$$\rho_0^{o,w,r} = \frac{\beta}{\alpha} + \frac{1}{\alpha}\left(\frac{p_0}{T}\right)$$

Thus, (E.1) defines a weakly compressible fluid. For the reservoir, we have

$$\mathbb{S} = S^w\phi\mathbb{S}^w + S^w\phi\mathbb{S}^w + (1-\phi)\mathbb{S}^r - S^w\phi\ln(S^w\phi) - S^o\phi\ln(S^o\phi) + (1-\phi)\ln(1-\phi) \tag{E.10}$$

where $p_w = p_o = p_r$ and $T_w = T_o = T_r$. By using equilibrium relations with the constitutive equations (E.9) and using p_0 for all constituents, we get

$$\left(\frac{\rho - \rho_0}{c}\right)_o = \left(\frac{\rho - \rho_0}{c}\right)_w = \left(\frac{\rho - \rho_0}{c}\right)_r \tag{E.11}$$

E.3 Derivation of Single-phase Flow Network Model

For the next step, we will substitute in the definition of the density $\mathbf{M} = \rho\phi\mathbf{V}$ and its derivative, where $\mathbf{M}$ and $\mathbf{V}$ are vectors and ρ and ϕ are diagonal matrices with the elements on the main diagonal being the densities or porosities of the grid blocks ρ_{ijk}, ϕ_{ijk} respectively. For the mass flow, we assume $\dot{\mathbf{M}} = \bar{\rho}\dot{\mathbf{V}}$ and thus a constant density along the flow connection according to the lumped parameter representation. We will assume the density in the flow connection to be an average value of the densities in the grid blocks it connects. We therefore introduce the following expression for a diagonal matrix $\bar{\rho}$ with diagonal elements of the form

$$\bar{\rho}_{ij,i+1j} = \frac{\rho_{ij} + \rho_{i+1j}}{2} \tag{E.12}$$

where matrix $\bar{\rho}$ is of the dimension of the total number of flows and can be decomposed into the submatrices for the total number of flows in each spacial direction. We choose a similar approach for the permeabilities in the gridblocks. Using Ohm's law, resistances can be combined serially according to

$$R_{total} = R_1 + R_2 \tag{E.13}$$

Similar to (E.12), we can define the elements of the permeability matrix $\mathbf{k}$ as the reciprocal of the flow resistance as

$$\bar{k}_{ij,i+1j} = \left(\frac{\frac{1}{k_{ij}} + \frac{1}{k_{i+1j}}}{2} \right)^{-1} \tag{E.14}$$

To describe the connection between inventory and potential, we will use an equation of state for the thermodynamics in the grid block $\rho = \rho(\mathbf{p}, \mathbf{T})$. Since we assume the reservoir to be isothermal, it follows $\rho = \rho(\mathbf{p})$. It follows

$$\frac{d(\phi\rho\mathbf{V})}{dt} = +\mathbf{A_x}\rho(\mathbf{p})\dot{\mathbf{V}}_\mathbf{x} + \mathbf{A_y}\rho(\mathbf{p})\dot{\mathbf{V}}_\mathbf{y} + \mathbf{Q}^* \tag{E.15}$$

using $\dot{\mathbf{V}}_\mathbf{x} = \Delta y \Delta z v_\mathbf{x}$, and $\dot{\mathbf{V}}_\mathbf{y} = \Delta x \Delta z v_\mathbf{y}$, we have

$$\frac{d(\phi\rho\mathbf{V})}{dt} = \mathbf{A_x}\rho\Delta y\Delta z v_\mathbf{x} + \mathbf{A_y}\rho\Delta x\Delta z v_\mathbf{y} + \mathbf{Q}^* \tag{E.16}$$

The Darcy velocities $v_\mathbf{x}$, $v_\mathbf{x}$, and $v_\mathbf{x}$ for the x and y-direction can now be substituted with Darcy's law $v_\mathbf{x} = -\frac{1}{\mu\Delta x}\mathbf{k_x}\Delta\mathbf{p_x}$

$$\frac{d(\phi\rho\mathbf{V})}{dt} = \frac{\Delta y\Delta z}{\Delta x\mu}\mathbf{A_x}\bar{\rho_x}\mathbf{k_x}\Delta\mathbf{p_x} + \frac{\Delta x\Delta z}{\Delta y\mu}\mathbf{A_y}\bar{\rho_y}\mathbf{k_y}\Delta\mathbf{p_y} + \mathbf{Q}^* \tag{E.17}$$

We can rewrite the accumulation term for constant volume V and using the compressibilities $c_l(p)$ and $c_r(p)$

$$\frac{d\rho\phi}{dt} = \rho\frac{\partial\phi}{\partial t} + \phi\frac{\partial\rho}{\partial t} = \left(\rho\frac{\partial\phi}{\partial p} + \phi\frac{\partial\rho}{\partial p}\right)\frac{dp}{dt} = \rho\phi(c_l + c_r)\frac{dp}{dt} = \rho\phi c_t(p)\frac{dp}{dt} \tag{E.18}$$

Using the compressibilities and Kirchhoff's voltage law (6.22), we transform (E.17) into

$$Vc_t(p)\rho\phi\frac{dp}{dt} = \frac{\Delta y\Delta z}{\Delta x\mu}\mathbf{A_x}\bar{\rho}\mathbf{k_x}\mathbf{A_x}^T\mathbf{p} + \frac{\Delta x\Delta z}{\Delta y\mu}\mathbf{A_y}\bar{\rho}\mathbf{k_y}\mathbf{A_y}^T\mathbf{p} + \mathbf{Q}^* \tag{E.19}$$

We derive the resulting nonlinear ordinary differential equation to

$$\mathbf{V}(\mathbf{p})\frac{d\mathbf{p}}{dt} = \mathbf{T}(\mathbf{p})\mathbf{p} + \mathbf{Q}^* \tag{E.20}$$

where

$$\begin{aligned}
\mathbf{V}(\mathbf{p}) &= \mathbf{Vc_t}(\mathbf{p})\rho(\mathbf{p})\phi(\mathbf{p}) && \text{(E.21)}\\
\mathbf{T} &= \mathbf{T_x} + \mathbf{T_y} + \mathbf{T_z} && \text{(E.22)}\\
\mathbf{T_x} &= \frac{\Delta y\Delta z}{\Delta x\mu}\mathbf{A_x}\bar{\rho}_x(p)\mathbf{k_x}\mathbf{A_x}^T && \text{(E.23)}\\
\mathbf{T_y} &= \frac{\Delta x\Delta z}{\Delta y\mu}\mathbf{A_y}\bar{\rho}_y(p)\mathbf{k_y}\mathbf{A_y}^T && \text{(E.24)}
\end{aligned}$$

The flow permeability $\bar{\mathbf{k}}$ and density $\bar{\rho}$ can be described in matrix form with the following matrix equations

$$\bar{\rho}\mathbf{I}^{n_f\times 1} = \mathbf{B}^T\rho \tag{E.25}$$

and

$$\bar{\mathbf{k}}^{-1}\mathbf{I}^{n_f\times 1} = \frac{1}{2}\mathbf{B}^T\mathbf{k}^{-1} \tag{E.26}$$

where $\mathbf{I}^{n_f\times 1} = [11...1]^T$ is a vector with ones for all elements of the dimension $n_f \times 1$. The reservoir model described in this section is a general description of the reservoir dynamics for single phase flow in two dimensions. The decomposition of the equation system into Kirchhoff laws and constitutive equations has advantages concerning stability and optimality analysis.

E.4 Derivation of Capacitive Constitutive Equations

We start with

$$\frac{d\rho_i^{o/w}\phi_i V_i^{o/w}}{dt} = \rho_i^{o/w}\phi_i\frac{dV_i^{o/w}}{dt} + \rho_i^{o/w}V_i^{o/w}\frac{d\phi_i}{dt} + \phi_i V_i^{o/w}\frac{d\rho_i^{o/w}}{dt} \tag{E.27}$$

We introduce the chain rule for the density and porosity

$$= \rho_i^{o/w}\phi_i\frac{dV_i^{o/w}}{dt} + \rho_i^{o/w}V_i^{o/w}\frac{\partial\phi_i}{\partial p_i}\frac{dp_i}{dt} + \phi_i V_i^{o/w}\frac{\partial\rho_i^{o/w}}{\partial p_i}\frac{dp_i}{dt} \tag{E.28}$$

using

$$c_i^{o/w} = \frac{\partial\rho_i^{o/w}}{\partial p_i}|_{T=const.}$$

where reservoir fluids are weakly compressible and $c_i^r = \frac{\partial\phi_i}{\partial p_i}|_{T=const.}$ (porous rock weakly compressible)

$$= \rho_i^{o/w}\phi(\frac{dV_i^{o/w}}{dt} + V_i^{o/w}(c_i^{o/w} + c_i^r)\frac{dp_i}{dt}) \tag{E.29}$$

E.5 Example: Six-gridblock model

E.5.1 Example: Six Grid Block Reservoir for Single Phase Flow

The application of the modeling framework is demonstrated on a simple single phase flow reservoir. The reservoir example consists of a reservoir with six grid blocks and two vertical wells as depicted in Fig. E.1. The six grid blocks have different permeabilities marked as high, low, and medium. We assume 2D reservoir flow and neglect flow in vertical direction as well as gravitational forces. The top left block contains an injection well and the bottom right block a production well. In a first step, we analyze the network structure of the model through a graph theoretical approach. We assume that the grid blocks are dynamic nodes in the reservoir network connected through flows and the boundaries are defined as the conditions at the injection and production well. The network model for

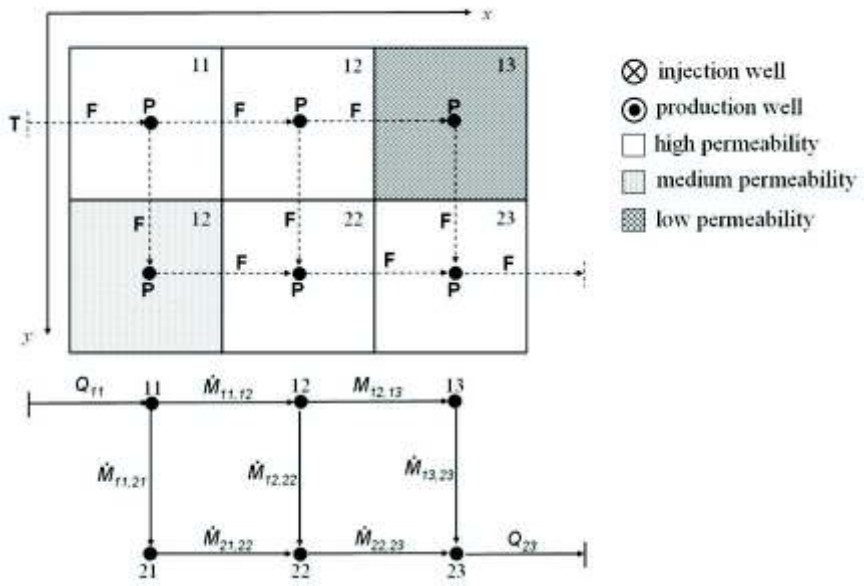

Figure E.1: The six grid block model displayed using graph nomenclature.

the six gridblock reservoir is given as conservation law (KCL), uniqueness condition (KVL), resistive constitutive equation, capacitive constitutive equation, and the initial condition.

Conservation law (KCL) for mass **M**:

$$\frac{d\mathbf{M}}{dt} = -\mathbf{A_x}\mathbf{M_x} - \mathbf{A_y}\mathbf{M_y} + \mathbf{LQ} \tag{E.30}$$

The uniqueness condition for the pressure **p** in decomposed form:

$$\Delta\mathbf{p_x} = \mathbf{A_x}^T\mathbf{p} \tag{E.31}$$

$$\Delta\mathbf{p_y} = \mathbf{A_y}^T\mathbf{p} \tag{E.32}$$

The resistive constitutive equations relating mass flow $\dot{\mathbf{M}}$ and pressure difference $\Delta\mathbf{p}$ given as a combination of Darcy's law $v_{\mathbf{x},\mathbf{y}} = -\frac{1}{\mu\Delta x,y}\bar{\mathbf{k}}_{\mathbf{x},\mathbf{y}}\Delta\mathbf{p}_{\mathbf{x},\mathbf{y}}$, definition for flow velocity $v_{\mathbf{x},\mathbf{y}} = \frac{\dot{\mathbf{V}}_{\mathbf{x},\mathbf{y}}}{\Delta xh}$ and density

$\dot{\mathbf{M}}_{\mathbf{x},\mathbf{y}} = \bar{\rho}_{\mathbf{x},\mathbf{y}} \dot{\mathbf{V}}_{\mathbf{x},\mathbf{y}}$:

$$\dot{\mathbf{M}}_{\mathbf{x}} = \frac{\Delta y h}{\Delta x \mu} \bar{\rho}_{\mathbf{x}} \bar{\mathbf{k}}_{\mathbf{x}} \Delta \mathbf{p}_{\mathbf{x}} \tag{E.33}$$

$$\dot{\mathbf{M}}_{\mathbf{y}} = \frac{\Delta x h}{\Delta y \mu} \bar{\rho}_{\mathbf{y}} \bar{\mathbf{k}}_{\mathbf{y}} \Delta \mathbf{p}_{\mathbf{y}} \tag{E.34}$$

For the capacitive constitutive equations, we are relating mass $\mathbf{M}$ and pressure $\mathbf{p}$ through the definition of the density $\mathbf{M} = \rho \phi \mathbf{V}$, and an equation of state for the density $\rho = \rho(p)$ and porosity $\phi = \phi(p)$.

$$\mathbf{M} = \rho(p)\phi(p)\mathbf{V} \tag{E.35}$$

The resulting differential equation system is given as

$$\mathbf{V}(\mathbf{p}) \frac{d\mathbf{p}}{dt} = \mathbf{T}(\mathbf{p})\mathbf{p} + \mathbf{Q}^* \tag{E.36}$$

where

$$\mathbf{V}(\mathbf{p}) = \mathbf{V}\mathbf{c}_{\mathbf{t}}(\mathbf{p})\rho(\mathbf{p})\phi(\mathbf{p}) \tag{E.37}$$

$$\mathbf{T} = \mathbf{T}_{\mathbf{x}} + \mathbf{T}_{\mathbf{y}} \tag{E.38}$$

$$\mathbf{T}_{\mathbf{x}} = \frac{\Delta y h}{\Delta x \mu} \mathbf{A}_{\mathbf{x}} \bar{\rho}_x(p) \mathbf{k}_{\mathbf{x}} \mathbf{A}_{\mathbf{x}}{}^T \tag{E.39}$$

$$\mathbf{T}_{\mathbf{y}} = \frac{\Delta x h}{\Delta y \mu} \mathbf{A}_{\mathbf{y}} \bar{\rho}_y(p) \mathbf{k}_{\mathbf{y}} \mathbf{A}_{\mathbf{y}}{}^T \tag{E.40}$$

$$\mathbf{Q}^* = \mathbf{L}\mathbf{Q} \tag{E.41}$$

The incident matrix for the system is given in Fig. E.2 If we assume that the reservoir fluid and rock is only weakly compressible, i.e. the compressibility c_t, density ρ, and porosity ϕ are not a function of the pressure p, then the accumulation matrix $\mathbf{V}$ and transmissibility matrix $\mathbf{T}$ reduce to constant matrices. Furthermore, the assumption of constant density for single phase flow implies that

	I^{6x6}						Q		M_x				M_y		
	M_{11}	M_{21}	M_{31}	M_{12}	M_{22}	M_{32}	Q_1	Q_2	$M_{11,21}$	$M_{21,31}$	$M_{12,22}$	$M_{22,32}$	$M_{11,12}$	$M_{21,22}$	$M_{31,32}$
M_{11}	1	0	0	0	0	0	-1	0	1	0	0	0	1	0	0
M_{21}	0	1	0	0	0	0	0	0	-1	1	0	0	0	1	0
M_{31}	0	0	1	0	0	0	0	0	0	-1	0	0	0	0	1
M_{12}	0	0	0	1	0	0	0	0	0	0	1	0	-1	0	0
M_{22}	0	0	0	0	1	0	0	0	0	0	-1	1	0	-1	0
M_{32}	0	0	0	0	0	1	0	1	0	0	0	-1	0	0	-1

Figure E.2: Incident matrix for the six grid block model.

the density in all grid blocks is equal and the density matrices reduce to scalars.

The reservoir example consists of a reservoir with six grid blocks and four vertical wells as depicted in Fig. E.3. The six grid blocks have different permeabilities marked as high low and medium. We assume 2D reservoir flow and neglect flow in vertical direction as well as gravitational forces. The left blocks contain injection wells and the right blocks production wells. The 6 grid block model is

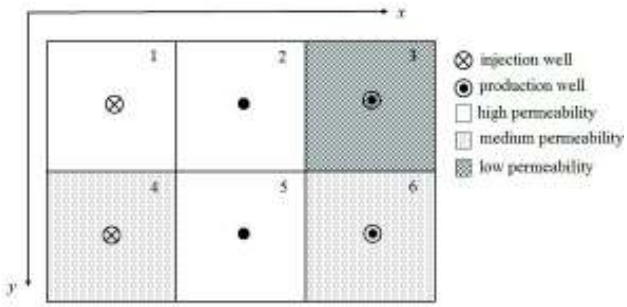

Figure E.3: Top view of a a reservoir model with six grid block and four wells.

given as:

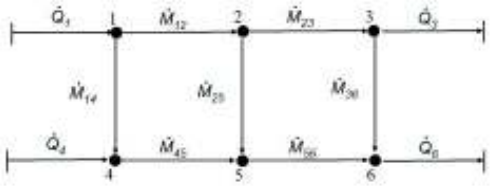

Figure E.4: The six grid block model displayed using graph nomenclature.

Mass balances oil/water (volume balances for constant density):

$$V\phi_1\frac{dS_1^{w,o}}{dt}+VS_1^{w,o}(c^r+c^{w,o})\phi_1\frac{dp_1}{dt} = -\dot{V}_{12}^{w,o}-\dot{V}_{14}^{w,o}+\dot{Q}_1^{w,o} \quad \text{(E.42)}$$

$$V\phi_2\frac{dS_2^{w,o}}{dt}+VS_2^{w,o}(c^r+c^{w,o})\phi_2\frac{dp_2}{dt} = \dot{V}_{12}^{w,o}-\dot{V}_{23}^{w,o}-\dot{V}_{25}^{w,o} \quad \text{(E.43)}$$

$$V\phi_3\frac{dS_3^{w,o}}{dt}+VS_3^{w,o}(c^r+c^{w,o})\phi_3\frac{dp_3}{dt} = \dot{V}_{23}^{w,o}-\dot{V}_{36}^{w,o}-\dot{Q}_3^{w,o} \quad \text{(E.44)}$$

$$V\phi_4\frac{dS_4^{w,o}}{dt}+VS_4^{w,o}(c^r+c^{w,o})\phi_4\frac{dp_4}{dt} = \dot{V}_{14}^{w,o}-\dot{V}_{45}^{w,o}+\dot{Q}_4^{w,o} \quad \text{(E.45)}$$

$$V\phi_5\frac{dS_5^{w,o}}{dt}+VS_5^{w,o}(c^r+c^{w,o})\phi_5\frac{dp_5}{dt} = \dot{V}_{45}^{w,o}+\dot{V}_{25}^{w,o}-\dot{V}_{56}^{w,o} \quad \text{(E.46)}$$

$$V\phi_6\frac{dS_6^{w,o}}{dt}+VS_6^{w,o}(c^r+c^{w,o})\phi_6\frac{dp_6}{dt} = \dot{V}_{36}^{w,o}+\dot{V}_{56}^{w,o}-\dot{Q}_6^{w,o} \quad \text{(E.47)}$$

Kirchhoff voltage law (implicit: $p^o = p^w$):

$$\Delta p_{ij} = p_i - p_j \quad \text{(E.48)}$$

Darcy's law:

$$\dot{V}_{12}^{w,o} = \frac{h\Delta y}{\mu^{w,o}} k_{12} k_{12}^{w,o} \frac{\Delta p_{12}}{\Delta x} \tag{E.49}$$

$$\dot{V}_{23}^{w,o} = \frac{h\Delta y}{\mu^{w,o}} k_{23} k_{23}^{w,o} \frac{\Delta p_{23}}{\Delta x} \tag{E.50}$$

$$\dot{V}_{45}^{w,o} = \frac{h\Delta y}{\mu^{w,o}} k_{45} k_{45}^{w,o} \frac{\Delta p_{45}}{\Delta x} \tag{E.51}$$

$$\dot{V}_{56}^{w,o} = \frac{h\Delta y}{\mu^{w,o}} k_{56} k_{56}^{w,o} \frac{\Delta p_{56}}{\Delta x} \tag{E.52}$$

$$\dot{V}_{14}^{w,o} = \frac{h\Delta x}{\mu^{w,o}} k_{14} k_{14}^{w,o} \frac{\Delta p_{14}}{\Delta y} \tag{E.53}$$

$$\dot{V}_{25}^{w,o} = \frac{h\Delta x}{\mu^{w,o}} k_{25} k_{25}^{w,o} \frac{\Delta p_{25}}{\Delta y} \tag{E.54}$$

$$\dot{V}_{36}^{w,o} = \frac{h\Delta x}{\mu^{w,o}} k_{14} k_{36}^{w,o} \frac{\Delta p_{36}}{\Delta y} \tag{E.55}$$

Saturation closure equation:

$$S_i^w + S_i^o = 1 \tag{E.56}$$

Permeabilities (geology):

$$k_{ij} = \frac{2}{\frac{1}{k_i} + \frac{1}{k_j}} \tag{E.57}$$

Relative permeabilities (saturation dependent):

$$k_{ij}^{ro,w} = \begin{cases} k_i^{o,w}, & \text{if } p_i \geq p_j \\ k_j^{ro,w}, & \text{if } p_i < p_j \end{cases} \tag{E.58}$$

$$k_i^{o,w} = k_0^{ro,w} \sigma_i^{n_w} \tag{E.59}$$

$$\sigma_i^w = \frac{S_i^w - S^{wc}}{1 - S^{or} - S^{wc}} \tag{E.60}$$

$$\sigma_i^o = \frac{S_i^o - S^{or}}{1 - S^{wc} - S^{or}} \tag{E.61}$$

$$\tag{E.62}$$

Injection wells (only water, $k_i^w = 1$, $k_i^0 = 0$):

$$\dot{Q}_1^w = J_1^w(p_{well,1} - p_1) \tag{E.63}$$

$$\dot{Q}_1^o = 0 \tag{E.64}$$

$$\dot{Q}_4^w = J_4^w(p_{well,4} - p_4) \tag{E.65}$$

$$\dot{Q}_4^o = 0 \tag{E.66}$$

$$\tag{E.67}$$

Production wells:

$$\dot{Q}_3^{w,o} = J_3^{w,o}(p_3 - p_{well,3}) \tag{E.68}$$

$$\dot{Q}_6^{w,o} = J_6^{w,o}(p_6 - p_{well,6}) \tag{E.69}$$

$$\tag{E.70}$$

Well index:

$$J_i^{w,o} = \frac{2\pi h k_1^{w,o} k_1}{\mu^{w,o}} \frac{1}{\ln\left(\frac{0.14\sqrt{\Delta x^2+\Delta y^2}}{r_{well,i}}\right)} \tag{E.71}$$

The degrees of freedom of the regarded reservoir model are the pressures at the wells ($p_{well,i}$). Tellegen's theorem gives the following redundant equations:

$$\begin{aligned}\sum_{i=1}^{6}(p_i(t_1)V\phi_i\frac{dS_i^w(t_2)}{dt} + p_i(t_1)VS_i^w(t_2)(c^r + c^{w,o})\phi_i\frac{dp_i(t_2)}{dt}) = -\sum_{FLOWS}\Delta p_{ij}(t_1)\dot{V}_{ij}^w(t_2) \\ + \sum_{WELLS}(p_{well,i}(t_1) - p_i(t_1))\dot{Q}_i^w(t_2) + \sum_{INJ}(p_{well,i}(t_1)\dot{Q}_i^w(t_2) - \sum_{PROD}(p_{well,i}(t_1)\dot{Q}_i^w(t_2)\end{aligned} \tag{E.72}$$

$$\sum_{i=1}^{6}(p_i(t_1)V\phi_i\frac{dS_i^o(t_2)}{dt}+p_i(t_1)VS_i^o(t_2)(c^r+c^{w,o})\phi_i\frac{dp_i(t_2)}{dt})=-\sum_{FLOWS}\Delta p_{ij}(t_1)\dot{V}_{ij}^o(t_2)$$
$$+\sum_{WELLS}(p_{well,i}(t_1)-p_i(t_1))\dot{Q}_i^o(t_2)+\sum_{INJ}(p_{well,i}(t_1)\dot{Q}_i^o(t_2)-\sum_{PROD}(p_{well,i}(t_1)\dot{Q}_i^o(t_2) \quad \text{(E.73)}$$

E.5.2 Parameters

Symbol	Parameter	number	unit
h	grid block height	20	m
$\Delta x, \Delta y$	grid block length/width	500	m
$V = \Delta x \Delta y h$	grid block volume	$5 \cdot 10^6$	m^3
μ^o	oil dynamic viscosity	$5 \cdot 10^{-4}$	Pas
μ^w	water dynamic viscosity	10^{-3}	Pas
k^{low}	low permeability (gb 3)	10^{-14}	m^2
k^{med}	medium permeability (gb 4,6)	10^{-13}	m^2
k^{high}	high permeability (gb 1,2,5)	10^{-12}	m^2
ϕ	porosity	0.3	-
r_{well}	well bore radius	0.114	m
p_r	initial reservoir pressure	$3 \cdot 10^7$	Pa
c^r	rock compressibility	10^{-8}	Pa^{-1}
c^o	oil compressibility	10^{-8}	Pa^{-1}
c^w	water compressibility	10^{-8}	Pa^{-1}
S^{or}	residual oil saturation	0.2	-
S^{wc}	connate water saturation	0.2	-
n^o	corey exponent, oil	1.0	-
n^w	corey exponent, water	1.0	-
k_0^o	endpoint relative permeability, oil	1.0	-
k_0^w	endpoint relative permeability, water	1.0	-

E.6 Proof of Stability for Reservoir Dynamics (Single Phase)

We begin with Tellegen's theorem:

$$\mathbf{W^T F} = 0$$

Since for each time t the vectors $\mathbf{W}$ and $\mathbf{F}$ lie in fixed orthogonal spaces, the identity

$$\dot{\mathbf{W}}^{\mathbf{T}}\mathbf{F} = 0 \tag{E.74}$$

is valid for the time derivatives of $\mathbf{W}$. We can decompose the identity into 3 terms

$$\frac{\partial}{\partial t}(\mathbf{p}^T\rho^{-1})\frac{d\mathbf{M}}{dt} - \frac{\partial}{\partial t}(\Delta\mathbf{p}^T\bar{\rho}^{-1})\dot{\mathbf{M}} + \frac{\partial}{\partial t}(\mathbf{p_Q}\rho_Q^{-1})\mathbf{Q} = 0 \tag{E.75}$$

storage, dissipative, and terminal terms. Using (E.74) in (E.76)

$$dP_w = -\frac{\partial}{\partial t}(\mathbf{p_Q}\rho_Q^{-1})\mathbf{Q} - \frac{\partial}{\partial t}(\Delta\mathbf{p}^T\bar{\rho}^{-1})\dot{\mathbf{M}} \tag{E.76}$$

and applying the product rule

$$dP_w = -\frac{\partial \mathbf{p_Q}}{\partial t}^T\rho_Q^{-1}\mathbf{Q} - \mathbf{p_Q}^T\frac{\partial \rho_Q}{\partial t}^{-1}\mathbf{Q} - \frac{\partial \mathbf{p}}{\partial t}^T\rho^{-1}\frac{d\mathbf{M}}{dt} - \mathbf{p}^T\frac{\partial \rho}{\partial t}^{-1}\frac{d\mathbf{M}}{dt} \tag{E.77}$$

For fixed (constant) well pressures $\mathbf{p}_Q$ and using $\Delta\mathbf{p}_Q = \mathbf{p}_Q$ the first well terms vanishes. Since the density $\rho = \rho(p)$ is a function of the pressure, thus, the densities at the wells are fixed as well and vanish. We use the chain rule $\frac{\partial\rho^{-1}}{\partial t} = \frac{\partial\rho}{\partial\mathbf{p}}\frac{dp}{dt}$

$$dP_w = -\frac{\partial \mathbf{p}}{\partial t}^T\rho^{-1}\frac{d\mathbf{M}}{dt} - \mathbf{p}^T\rho^{-1}\frac{\partial\rho}{\partial\mathbf{p}}\frac{d\mathbf{p}}{dt}\frac{d\mathbf{M}}{dt} \tag{E.78}$$

Substituting the compressibility $\mathbf{c_l} = \rho^{-1}\frac{\partial\rho}{\partial\mathbf{p}}$ gives

$$dP_w = -\frac{\partial \mathbf{p}}{\partial t}^T\rho^{-1}\frac{d\mathbf{M}}{dt}(1 - \mathbf{p}^T\mathbf{c_l}) \tag{E.79}$$

For the reservoir to converge to a stable and unique solution, (E.79) has to be negative for all times. The term $\frac{\partial \mathbf{p}}{\partial t}^T \rho^{-1} \frac{d\mathbf{M}}{dt}$ is positive, if the product of $\frac{\partial \mathbf{p}}{\partial t}$ and $\frac{d\mathbf{M}}{dt}$ is positive, i.e. $\mathbf{M} = f(\mathbf{p})$ has to be monotonically increasing. For the term $1 - \mathbf{p^T c_l}$, we observe that for weakly compressible fluids $\mathbf{p^T c_l} \ll 1$ and thus we have stable convergence.

E.7 Lyapunov stability of reservoir

We begin by defining Lyapunov stability:

Definition 23. *Consider an autonomous nonlinear dynamical system*

$$\dot{\mathbf{x}} = f(\mathbf{x}) \tag{E.80}$$

then we can consider a function $V(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}$ *such that*

$$V(\mathbf{x}) \geq 0 \tag{E.81}$$

and

$$\frac{dV(\mathbf{x})}{dt} < 0 \tag{E.82}$$

a Lyapunov candidate function and the systems is asymptotically stable in the sense of Lyapunov.

We can define a Lyapunov candidate function as

$$G_R^* = \int^{\mathbf{W_R}} \mathbf{F_R}^T d\mathbf{W_R} = \int^{\bar{\rho}^{-1}\Delta\mathbf{p}} \dot{\mathbf{M}}^T d(\bar{\rho}^{-1}\Delta\mathbf{p})$$

as a function of flow and potential difference variables. Using the Kirchhoff laws and the resistive (Darcy's law) and capacitive (equation of state) constitutive equations, we can transform the

Lyapunov candidate function into a function of either the extensive or intensive state variables, i.e. masses $V(\mathbf{M})$ or pressures $V(\mathbf{p})$ of the gridblocks. We will continue with the masses as state variable.

If there exists an equilibrium point $\mathbf{M}^*$ then there always exists a coordinate transformation $\mathbf{x} = \mathbf{M} - \mathbf{M}^*$ such the equilibrium point of the new coordinate lies in the origin $\mathbf{x}^* = \mathbf{0}$.

For strictly monotonous resistive constitutive equations, the co-content is positive definite and radially unbounded, since

$$\|\mathbf{M}\| \to \infty \Rightarrow \int^{\bar{\rho}^{-1}\Delta\mathbf{p}} \dot{\mathbf{M}}^T d(\bar{\rho}^{-1}\Delta\mathbf{p}) \to \infty$$

We can show that

$$\mathbf{V}(\mathbf{M}) = \frac{\partial}{\partial t}(\Delta\mathbf{p}^T\bar{\rho}^{-1})\dot{\mathbf{M}} < 0$$

for $\forall \mathbf{M} \in \mathbb{R}^n \setminus \{\mathbf{0}\}$. Using theorem 26, it follows that the time derivative of the Lyapunov candidate function is negative definite if the equation of state is strictly monotonous and the the product of compressibility and pressure is much smaller than 1.

E.8 Corey model and Upstream Weighting

To model the saturation dependency of the permeabilities, we consider the Corey model:

$$\begin{aligned}
k_{ij}^{ro,w} &= k_0^{ro,w}\sigma_{ij}^{n_w} && \text{(E.83)}\\
\sigma_{ij}^{w} &= \frac{S_{ij}^{w} - S^{wc}}{1 - S^{or} - S^{wc}} && \text{(E.84)}\\
\sigma_{ij}^{o} &= \frac{S_{ij}^{o} - S^{or}}{1 - S^{wc} - S^{or}} && \text{(E.85)}\\
\mathbf{S}^w + \mathbf{S}^o &= 1 && \text{(E.86)}\\
& && \text{(E.87)}
\end{aligned}$$

where $k_0^{r,w}$ and $k_0^{r,o}$ are the end-point relative permeabilities, n_w and n_o are the Corey exponents, S^{wc} is the connate water saturation and S^{or} is the residual oil saturation. The permeabilities for flows are are taken through upstream weighting:

$$k^{ro,w} = \begin{cases} k_{ij}^{ro,w}, & \text{if } p_{ij} \geq p_{i+1j} \\ k_{i+1j}^{ro,w}, & \text{if } p_{ij} < p_{i+1j} \end{cases} \tag{E.88}$$

E.9 Proof of Dissipative Properties of Two-phase Subsurface Flow

We can decompose the constitutive equations of the form $\mathbf{AF} = \mathbf{0}$ into

$$\frac{d\mathbf{V}^o}{dt} = -\mathbf{A}\dot{\mathbf{V}}^o - \mathbf{L}\dot{\mathbf{V}}_\mathbf{T}^o \tag{E.89}$$

$$\frac{d\mathbf{V}^w}{dt} = -\mathbf{A}\dot{\mathbf{V}}^w - \mathbf{L}\dot{\mathbf{V}}_\mathbf{T}^w \tag{E.90}$$

Also, we have

$$\frac{dE}{dt} = \frac{\partial E}{\partial \mathbf{V}^o}\frac{dV^o}{dt} + \frac{\partial E}{\partial \mathbf{V}^w}\frac{dV^w}{dt} \tag{E.91}$$

The dissipation inequality in differential form is given as

$$0 \leq \frac{dE}{dt} \leq \phi_E(\dot{\mathbf{V}}_\mathbf{T}, \mathbf{p_T}) \tag{E.92}$$

using (E.89), (E.89), and (E.91).

$$0 \leq \frac{\partial E}{\partial \mathbf{V}^o}\mathbf{A}\dot{\mathbf{V}}^o + \frac{\partial E}{\partial \mathbf{V}^w}\mathbf{A}\dot{\mathbf{V}}^w \leq \phi_E(\dot{\mathbf{V}}_\mathbf{T}, \mathbf{p_T})$$

It follows that the reservoir is passive, if

$$\frac{\partial E}{\partial \mathbf{V}^o}\mathbf{A}\dot{\mathbf{V}}^o + \frac{\partial E}{\partial \mathbf{V}^w}\mathbf{A}\dot{\mathbf{V}}^w \leq \mathbf{p_T}^T\dot{\mathbf{V}}_\mathbf{T} - \beta_1\dot{\mathbf{V}}_\mathbf{T}^T\dot{\mathbf{V}}_\mathbf{T} - \beta_2\mathbf{p_T}^T\mathbf{p_T}$$

If we define a storage function such as the availability [2]

$$E = (\mathbf{p}^* - \mathbf{p})^T \mathbf{V}^{\mathbf{w}} + (\mathbf{p}^* - \mathbf{p})^T \mathbf{V}^{\mathbf{o}} \tag{E.93}$$

which is homogeneous and degree one, then we can show the dependence on the flow connections. Using Tellegen's theorem

$$0 \leq -(\dot{\mathbf{V}}^{\mathbf{w}})^T \Delta\mathbf{p} - (\dot{\mathbf{V}}^{\mathbf{o}})^T \Delta\mathbf{p} - \dot{\mathbf{V}}_{\mathbf{T}}^T p_T \leq \phi_E(\dot{\mathbf{V}}_{\mathbf{T}}, \mathbf{p}_{\mathbf{T}})$$

it follows

$$(\dot{\mathbf{V}}^{\mathbf{w}})^T \Delta\mathbf{p} (\dot{\mathbf{V}}^{\mathbf{o}})^T \Delta\mathbf{p} \geq \beta_1 \dot{\mathbf{V}}_{\mathbf{T}}^T \dot{\mathbf{V}}_{\mathbf{T}} - \beta_2 \mathbf{p}_{\mathbf{T}}{}^T \mathbf{p}_{\mathbf{T}} \geq 0 \tag{E.94}$$

as a condition of passivity. The reservoir is strictly input passive, if $\beta_2 > 0$ (for the pressures $\mathbf{p}_{\mathbf{T}}$ being the well input variables) and strictly output passive for $\beta_1 > 0$ (for the flows $\dot{\mathbf{V}}$ being the terminal output variables) and vice versa. If (E.94) holds, then the system is globally asymptotically stable and has a unique stationary point.

E.10 Optimization Problem for Closed-loop Reservoir Management

The optimization problem for the displacement efficiency in a petroleum reservoir can modeled so that

$$\min_{\mathbf{p_u},\mathbf{q_u}} \quad \Phi(\mathbf{S}^w,\mathbf{S}^o,\mathbf{p},\mathbf{q_u},\mathbf{p_u}) \tag{E.95}$$

$$s.t. \quad V\phi\frac{d\mathbf{S}^w}{dt}+V\mathbf{S}^{wT}\phi(\mathbf{c}^r+\mathbf{c}^w)\frac{d\mathbf{p}}{dt}=-\mathbf{T}^w(\mathbf{S}^w)\mathbf{p}+\mathbf{Q}^w(\mathbf{S}^w,\mathbf{q_u},\mathbf{p_u}) \tag{E.96}$$

$$V\phi\frac{d\mathbf{S}^o}{dt}+V\mathbf{S}^{oT}\phi(\mathbf{c}^r+\mathbf{c}^o)\frac{d\mathbf{p}}{dt}=-\mathbf{T}^o(\mathbf{S}^o)\mathbf{p}+\mathbf{Q}^o(\mathbf{S}^o,\mathbf{q_u},\mathbf{p_u}) \tag{E.97}$$

$$\mathbf{S}^w+\mathbf{S}^o=1 \tag{E.98}$$

$$\text{Initial conditions: } \mathbf{S}^w(0)=\mathbf{S}^w_0,\mathbf{S}^w(0)=\mathbf{S}^o_0,\mathbf{p}(0)=\mathbf{p}_0 \tag{E.99}$$

$$\mathbf{p}^{LB}\leq\mathbf{p_u}\leq\mathbf{p}^{UB},\ \mathbf{q}^{LB}\leq\mathbf{q_u}\leq\mathbf{q}^{UB} \tag{E.100}$$

where $\mathbf{p_0}$ and the saturations $\mathbf{S^w_0}$ and $\mathbf{S^o_0}$ are the initial conditions for the state variables which are decision variables in the optimization problem along with states throughout the time horizon. The flows $\mathbf{q_u}$ and pressures $\mathbf{p_u}$ at the wells serve as control variables. The objective of the water injection process is generally to maximize the profit for the amount of recovered oil while minimizing production cost. It is common to maximize the following objective function

$$\Phi=\int_0^T(\sum_{n_{PROD}}r_{oil}(t)q_{oil}-\sum_{n_{PROD}}c_{prod,water}(t)q_{water}-\sum_{n_{INJ}}c_{inj,water}(t)q_{inj,water})(1+d(t))^{-t})dt \tag{E.101}$$

where the costs for water injection and production are subtracted from the revenues for produced oil multiplied by a discounting factor. It is apparent that in this practical setting, it remains an open question as to how to predict or fix the production horizon. In practice, field production is stopped as soon as operations becomes permanently unprofitable, i.e., the produced fluid is mostly water. A

simplified policy commonly used in the upstream industry is the reactive strategy, where production is stopped for each production well, when a certain water-to-oil ratio is exceeded. We derive a set of fundamental physical principles and objectives towards determining simple decentralized policies for the decision making in which the level of optimality can be increased from the simple reactive strategy towards including feedback from different sources of information from subsurface flow measurements.