Optimality of Process Networks. ⋆

Michael R. Wartmann * **B. Erik Ydstie** *

* *Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, USA (e-mail: wartmann@cmu.edu, ydstie@cmu.edu).*

Abstract: In this paper we show that conservation laws for extensive quantities and the second law of thermodynamics lead to conditions for stability and optimality of a process network. Interconnections among nodes are represented through connectivity matrices and network graphs. A generalized version of Tellegen's theorem from electrical circuit theory plays a central role in deriving the objective function of the regarded dynamic process networks. The application of irreversible thermodynamics lead to stability and optimality results based on the co-content and content of the regarded process networks. The principle is illustrated in a pipeflow example.

Keywords: dissipation, network theory, irreversible thermodynamics, distributed control, passivity theory.

1. INTRODUCTION

The complexity of process systems arises from the variety of how simple subunits are connected (Hangos et al. (1999)). A crucial component in modeling process systems is therefore to understand how connections between the subunits lead to complex system behavior. Ydstie and Alonso (1997) developed a theoretical framework providing a link between passivity theory and physics using the second law of thermodynamics. They discussed the need to develop passivity based control techniques which focus on input-output properties of the systems. An understanding for complex behavior can then be derived from macroscopic thermodynamic constraints instead of microscopic equations and the complexity that results from using very detailed models can be reduced. Jillson and Ydstie (2007) developed a topological result similar to Tellegen's theorem of electrical circuit theory and passivity theory to derive sufficient conditions under which a network is stabilized using decentralized feedback. The theory shows that it is possible to control very complex networks of process systems without actually modeling the thermodynamics and kinetics explicitly. This is due to inherent passivity properties that follow from the second law of thermodynamics. The conditions for passivity can be checked in a distributed manner. In this work, we will explore if similar ideas can be applied for optimization.

We extend the approaches in Ydstie and Alonso (1997); Jillson and Ydstie (2007) to provide an organizational framework for treating complex process systems concerning optimality using ideas from network theory. The formalism of network theory has been particularly successful for modeling and control of dynamic systems in electrical engineering applications. Classically, electrical circuit theory is not considered an application of non-equilibrium thermodynamics. Nevertheless, electrical circuits are typical irreversible thermodynamic systems. The formalism developed in electrical circuit theory was extended to general thermodynamic systems by Oster et al. (1971); Peusner (1986). In particular the application to complex biological systems has been carried out successfully by Oster and Desoer (1971); Mickulecky (2001). In this paper, we apply the formalism of network theory to describe connected process systems. Network theory brings thermodynamics a degree of mathematical rigor and allows to unify ideas from non-equilibrium thermodynamics, dynamic system theory and control. In the context of dissipativity of process systems, network theory facilitates the extension of irreversible thermodynamics by the system's topological description which is an important part of the dynamic behavior. Looking at mathematical models of many dynamic physical systems, we can identify a certain inherent structure. We can separate the network model into a kinematic structure which addresses the topology of the system and a dynamical structure (Oster and Desoer (1971)). The connectivity properties of the system describe the physical processes where the dynamical structure defines the relationships between the state variables. The paper is organized as follows: In Section 2, we define the type of process systems and describe the connection to network theory, in Section 3, we describe fundamental topological properties of the regarded process networks. In Section 4 and 5, we elaborate the concepts of stability and optimality for the regarded systems and present a pipeflow example to illustrate our findings in Section 6.

2. PROCESS NETWORKS

Process networks are written as a collection of interconnected sub-systems

$$\dot{x}_i = F(x_i) + \sum_{j=0, j\neq i}^{n} G(u_i, x_i, x_j), \quad i = 0, ..., n \tag{1}$$

$$y_i = H(x_i) \tag{2}$$

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

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connected with other sub-systems, and the output function H relates the state of the system to the measurement functions y_i. The functions u_i represent the manipulated variables. The functions F, G, H are all differentiable at least once. The state of the entire network is given by the vector $x = (x_0^T, x_1^T, ..., x_n^T)^T$.

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 process system is modeled as the reduced system without the reference sub-system. Its state is given by the vector $x = (x_1^T, ..., x_n^T)^T$. The interactions with the exo-system are then established through the boundary conditions.

The network form, as illustrated in Figure 1 is convenient when we model systems with a graph structure. In such systems the interactions between the sub-systems depend on the state of the sub-system itself and the state of its immediate neighbors. Not all dynamical systems can be decomposed in this fashion. However, many large scale systems have sparse interconnections and they can be modeled compactly as networks of sub-systems with interconnections. It is also easy to see that many physical systems, especially those that satisfy the principle of local action, can be decomposed in the manner shown in (1).

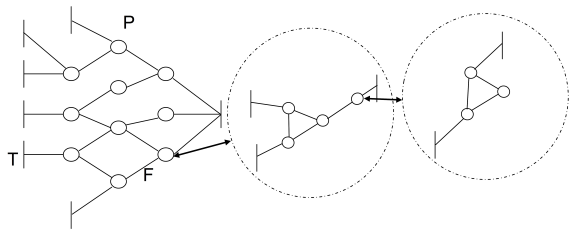

Fig. 1. Graphical network representation: Topological structure of a network consisting of nodes, terminals, and flows. Nodes can contain subgraphs and give rise to a hierarchical, multiscale structure.

We define the inventory Z of a sub-system or a group of systems to be 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. 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.

By referring to (1) and using continuity we derive the conservation law

$$\frac{dZ_i}{dt} = p_i(x_i) + \sum_{j=1, j\neq i}^{n} f_{ij}(u) \tag{3}$$

The *drift* $p_i(x_i) = \frac{\partial Z(x_i)}{\partial x_i} F(x_i)$ measures the rate of production and the function $f_{ij}(u) = \frac{\partial Z(x_i)}{\partial x_i} G(u, x_i, x_j)$ 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.

Definition: Let X_0 be a subset of state-space. An inventory defined by (3) is said to have the

(1) *Clausius-Planck property* if $p(x) > 0$ for x not in X_0
(2) *Conservation property* if $p(x) = 0$ for all x not in X_0
(3) *Dissipation inequality* if $p(x) < 0$ for x not in X_0

The set X_0 associated with the dissipative action ϕ is called the set of *passive states*.

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

- If, for all $(\upsilon_i, \upsilon_j) \in \epsilon(\mathbf{G})$, the branch $(\upsilon_j, \upsilon_i) \in \epsilon(\mathbf{G})$ 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.

Definition 1. A network of nodes $P_i, i = 1, ..., n_p, n_p + 1, ..., n_v$ consisting of nodes and terminals interconnected through branches $E_i, i = 1, ..., n_f$ with topology defined by the graph

$$\mathbf{G} = (\mathbf{E}, \mathbf{P})$$

is called a *process network* if its interconnection structure is described by a directed graph and we have

(1) **First law:** There exists an inventory E (the energy) which satisfies the conservation property
(2) **Second law:** There exists an inventory S (the entropy) which satisfies the Clausius-Planck property

We now develop a compact description of the topology of the network by introducing the incidence matrix.

Definition 2. The $n_t \times n_f$ matrix $\mathbf{A_a}$ is called incidence matrix for the matrix elements a_{ij} being

$$a_{ij} = \begin{cases} 1, & \text{if flow } j \text{ leaves node } i \\ -1, & \text{if flow } j \text{ enters node } i \\ 0, & \text{if flow } j \text{ is not incident with node } i \end{cases}$$

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

The connections between nodes through branches can be uniquely defined using the incident matrix $\mathbf{A}$. The conservation laws (3) can now be written

$$\mathbf{AF} = \mathbf{0} \tag{4}$$

for the node-to-branch incident matrix $\mathbf{A}$, where $\mathbf{F^T} = [\frac{dZ_1}{dt}, \frac{dZ_2}{dt}, .., \frac{dZ_t}{dt}, f_{12}, f_{13}..f_{n_{t-1}, n_t}, p_1, .., p_t]$. The flows f_{ij} represent connections between two nodes i.e. f_{ij} connects node i to node j, p_i denotes sources or sinks. The direction of the flows are defined according to the directionality

established in the graph. We now define a vector $\mathbf{W}$ so that

$$\mathbf{W} = \mathbf{A^T w} \tag{5}$$

where $\mathbf{W}$ are the potential differences across flow connections. The variables w are conjugate to Z if they are related via the Legendre transform of a convex potential like the entropy.

A dual structural representation can be derived using mesh analysis (the analysis developed above, which is based on the conservation laws, is called node analysis). Mesh analysis is counter-intuitive in process control applications but frequently used for electrical circuit analysis. When introducing stability and optimality concepts in this work, we will focus on describing the primal problem and its implications but refer to the dual mesh-based problem as proving the equivalent dual case.

2.1 Constitutive Relations

Constitutive equations relate efforts and flows (resistive), flows and displacements (capacitive), and efforts and fluxes (inductive). The constitutive equations describe energy dissipating, irreversible processes (resistive) or energy storing, reversible processes. The constitutive equations define the type of energetic transaction inside the process system or between the process system and the environment. The three main types can be described as

- Capacitive constitutive equation: storage of potential energy, $W = f_C(Z)$
- Inductive constitutive equation: storage of kinetic energy, $p = f_L(W)$
- Resistive constitutive equation: dissipation of energy, $F = f_R(W)$

In the context of process networks, storage of energy usually occurs through capacitive elements. In this work, inductive constitutive equations are neglected due to the fact that we focus on chemical processes or chemical process plants in which inertial effects in mass flow and thus accumulation of kinetic energy are not a significant contributor to the energy balance.

3. TOPOLOGICAL RESULTS, CONTENT AND CO-CONTENT

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 superscript a and denote variables in the other network with superscript b. Using the conservation laws (4) we can then write $\mathbf{W^{a}}^T\mathbf{F^b} = (\mathbf{A}^T\mathbf{w^a})^T\mathbf{F^b} = \mathbf{w^a}^T\mathbf{A}\mathbf{F^b} = 0$. The equality

$$\mathbf{W^{a}}^T\mathbf{F^b} = 0$$

is often called *Tellegen's theorem.*

Without the reference system Tellegen's theorem is written

$$\mathbf{w^b}^T\frac{d\mathbf{Z^a}}{dt} = -\mathbf{W_R^b}^T\mathbf{F_R^a} - \mathbf{w_T^b}^T\mathbf{F_T^a} - \mathbf{w^b}^T\mathbf{p^a} \tag{6}$$

The term of the left hand side is called the storage. The three terms on the right refer to power dissipation due to transportation, supply from the exo-system through the terminals, and dissipation by production respectively.

If we consider a single network ($a = b$), then we can drop the superscript and we get the common form $\mathbf{W}^T\mathbf{F} = 0$ which represents a powerbalance. If Z represents the energy then we get the classical energy balance for the network. The "balance of entropy dissipation" results if we let one inventory correspond to the thermodynamic entropy defined so that

$$S = k_B \ln \Omega(x)$$

It is important to note that the fundamental equation gives a definition of the classical entropy in terms of extensive and intensive variables through the Pfaffian

$$TdS = dU + PdV - \sum_{i=1}^{n_c} \mu_i dN_i$$

Tellegen's theorem applied to the primal (extensive variable) vector $Z = (U, V, N_1, .., N_n)$ and its Legendre dual (intensive variable) vector $w = (1, P, \mu_1, .., \mu_n)/T$ then gives

$$\dot{S} = \mathbf{W_R}^T\mathbf{F_R} + \mathbf{w_T}^T\mathbf{F_T} + \mathbf{w}^T\mathbf{p}$$

where we used the fundamental equation and (6). The term $p_S = \mathbf{F_R}^T\mathbf{W_R} + \mathbf{w^T p}$ is called the rate of entropy generation.

We define the content of the network as the integral

$$G_R = \int_0^{\mathbf{F_R}} \mathbf{W_R}^T d\mathbf{F_R} + \int_0^{\mathbf{p}} \mathbf{w}^T d\mathbf{p} \tag{7}$$

The co-content is given as

$$G_R^* = \int_0^{\mathbf{W_R}} \mathbf{F_R}^T d\mathbf{W} + \int_0^{\mathbf{w}} \mathbf{p}^T d\mathbf{w} \tag{8}$$

By integration by parts and proper choice of the constant p^* (the constant of integration) we see that

$$G_R + G_R^* = p_S \geq 0$$

The second law dictates that the inequality holds (positive entropy production).

4. STABILITY OF PROCESS NETWORKS

In this section we derive a stability result using a combination of Tellegen's theorem and the co-content as a line integral. First, we note that Tellegen's theorem shows that for each time t the vectors $\mathbf{W}$ and $\mathbf{F}$ lie in fixed and orthogonal spaces. The identity $\dot{\mathbf{W}}^T\mathbf{F} = 0$ is therefore valid for all t and by taking out the sub-system which represent the exo-system we can write as before

$$\dot{\mathbf{Z}}^T\dot{\mathbf{w}} = -\mathbf{F_R^T}\dot{\mathbf{W}}_\mathbf{R} - \mathbf{F_T^T}\dot{\mathbf{w}}_\mathbf{T} - \mathbf{p_T^T}\dot{\mathbf{w}} \tag{9}$$

Due to the concavity of the entropy function we know that there exists a matrix $\mathbf{M} \geq 0$ so that $d\mathbf{w} = \mathbf{M}d\mathbf{Z}$, hence

$$\dot{\mathbf{Z}}^T\dot{\mathbf{w}} = \dot{\mathbf{Z}}^T M\dot{\mathbf{Z}} \geq 0$$

We can also write the co-content as a line integral

$$G_R^* = \int^t (\mathbf{F_R}^T\dot{\mathbf{W}}_\mathbf{R} + \mathbf{p}^T\dot{\mathbf{w}})dt \geq 0$$

Hence, by integrating (9) we get

$$\int_0^t \dot{\mathbf{Z}}^T M\dot{\mathbf{Z}}dt = -G_R^* - \mathbf{F_T^T}\dot{\mathbf{w}}_\mathbf{T}$$

The contribution due the terminal potentials vanish if $\dot{\mathbf{w}}_\mathbf{T} = 0$ and it follows that G^* is integrable and subject the condition of uniform continuity we conclude that G^* converges which implies that $\dot{\mathbf{w}}$ converges to zero.

5. OPTIMALITY OF PROCESS NETWORKS

Maxwell (1892) formulated the minimum heat theorem which states that for linear resistive electrical circuits driven by constant power sources, the flows distribute themselves in a way as to minimize the heat that is dissipated through the resistive elements. Prigogine (1947) observed that the theorem can be generalized to thermodynamic systems with the entropy production σ_S being minimized at steady state. Based on Tellegen's theorem and the content and co-content, we can propose an optimization problem that allows us to find the steady state and dynamic trajectory of a dynamic process network.

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

$$G = \sum_{i=1}^{b} \int^{F_i} W_i dF_i = \int^{\mathbf{F}} \mathbf{W}^T d\mathbf{F} \tag{10}$$

and the extended co-content:

$$G^* = \sum_{i=1}^{b} \int^{W_i} F_i dW_i = \int^{\mathbf{W}} \mathbf{F}^T d\mathbf{W} \tag{11}$$

The extended content G and co-content G^* represent the sum of contents and co-contents for all branches i.e. reversible, irreversible, production and terminal flow connections of the network.

Lemma 3. For the network content G and the co-content G^*

$$G^*(\mathbf{W}) = \mathbf{W}^T\mathbf{F} - G(\mathbf{F}) \tag{12}$$

Equation (12) is a special form of Tellegen's theorem and can be used to do a variable change corresponding to a Legendre transformation.

Proof. The relation follows directly from integration by parts.

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

$$G + G^* = 0$$

Proof. Using Tellegen's theorem and Lemma 3, the result follows immediately.

Definition 5. The following set of equations defines the process system:

$$\mathbf{AF} = \mathbf{0} \tag{13}$$
$$\mathbf{W} = \mathbf{A^T w} \tag{14}$$
$$\mathbf{F_R} = \Lambda(\mathbf{W_R}) \tag{15}$$
$$\mathbf{Z} = \mathbf{C w_C} \tag{16}$$
$$\mathbf{F_R} = \mathbf{F} - \mathbf{F_S} \tag{17}$$
$$\mathbf{W_R} = \mathbf{W} - \mathbf{W_S} \tag{18}$$
$$\mathbf{F_S} = \mathbf{F_T} \tag{19}$$
$$\mathbf{W_S} = \mathbf{W_T} \tag{20}$$
$$\mathbf{Z(0)} = \mathbf{Z_0} \tag{21}$$

The first two equations (13) and (14) are the Kirchhoff relations for process networks. Equations (15) are the resistive constitutive equations with Λ being a matrix function and (16) are the capacitive constitutive equations.

We introduced the variables $\mathbf{F_R}$ and $\mathbf{W_R}$ which facilitate writing the resistive constitutive equations in a compact way. The variables $\mathbf{F_R}$ and $\mathbf{W_R}$ allow us to include the terminals as sources or sinks through (19) and (20) for both, terminals where we have the function of the flows $\mathbf{F_T}$ or the potentials $\mathbf{W_T}$ given. For simplicity, we assume the terminal conditions as constant over time. The last equation (21) constitutes the initial conditions for the inventories $\mathbf{Z}$.

The set of equations can be transformed into a system of nonlinear differential algebraic equations (DAE) of the form

$$\frac{d\mathbf{Z}}{dt} = \mathbf{A}(\mathbf{Z}) + \mathbf{B}^{\mathbf{Z}}_{\mathbf{F}}(\mathbf{F}^{\mathbf{input}}_{\mathbf{T}}) + \mathbf{B}^{\mathbf{Z}}_{\mathbf{W}}(\mathbf{W}^{\mathbf{input}}_{\mathbf{T}}) \tag{22}$$
$$\mathbf{W}^{\mathbf{output}}_{\mathbf{T}} = \mathbf{C}^{\mathbf{W}}(\mathbf{Z}) + \mathbf{D}^{\mathbf{W}}_{\mathbf{F}}(\mathbf{F}^{\mathbf{input}}_{\mathbf{T}}) + \mathbf{D}^{\mathbf{W}}_{\mathbf{W}}(\mathbf{W}^{\mathbf{input}}_{\mathbf{T}}) \tag{23}$$
$$\mathbf{F}^{\mathbf{output}}_{\mathbf{T}} = \mathbf{C}^{\mathbf{F}}(\mathbf{Z}) + \mathbf{D}^{\mathbf{F}}_{\mathbf{W}}(\mathbf{W}^{\mathbf{input}}_{\mathbf{T}}) + \mathbf{D}^{\mathbf{F}}_{\mathbf{F}}(\mathbf{F}^{\mathbf{input}}_{\mathbf{T}}) \tag{24}$$

where nonlinearities are introduced through the constitutive equations. In this dynamic system, each terminal has an input and an output variable. The set of differential equations (22) determines the trajectories of $\mathbf{Z}$ and represent a state space system. The algebraic constraints (23) and (24) compute the output variables at the terminals from the input variables and the state $\mathbf{Z}$.

To find the stationary solutions of the system, we need to solve the set of equations

$$\mathbf{AF} = \mathbf{0} \tag{25}$$
$$\mathbf{W} = \mathbf{A^T w} \tag{26}$$
$$\mathbf{F} - \mathbf{F_T} = \Lambda(\mathbf{W} - \mathbf{W_T}) \tag{27}$$

with the three main sets of constraints: Conservations laws, uniqueness conditions, and the constitutive equations. The inventories and capacitive constitutive equations are only relevant for the dynamic case.

In the following theorem, we introduce the connection between content, co-content and the Kirchhoff laws, and present how duality of the free variables plays a crucial role for the optimization problem that is solved when a process network converges to a steady state solution. The constitutive equations are not directly involved as they are not relevant for the topological properties of the process network.

Theorem 6. For the optimization problem

$$\min_{\mathbf{w}} G^* = \int_0^W \mathbf{F}^T d\mathbf{W} \tag{28}$$
$$s.t. \quad \mathbf{W} = \mathbf{A^T w} \tag{29}$$
$$\mathbf{F} = \Lambda(\mathbf{W}) \tag{30}$$

with the cocontent G^* as objective function, the uniqueness conditions, and resistive constitutive equations as constraints, the solution exhibits a set of equations consisting of the uniqueness condition, the conservation laws, and the constitutive equations. The Langrange multipliers of the optimization problem are the network flow variables $\mathbf{F}$.

Proof. Starting with equations (28) - (30), we first substitute the constitutive equations (30) into the objective function (28) to eliminate the flow variables $\mathbf{F}$. The Lagrange function of the resulting optimization problem is

$$\min L(\mathbf{W}, \mathbf{w}, \lambda) = \int_0^W \Lambda(\mathbf{W})^T d\mathbf{W} + \lambda^T(\mathbf{A^T w} - \mathbf{W}) \quad (31)$$

First order conditions:

$$\frac{\partial L}{\partial \mathbf{W}} = \Lambda(\mathbf{W}) - \lambda = \mathbf{0} \quad (32)$$

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{A}\lambda = \mathbf{0} \quad (33)$$

$$\frac{\partial L}{\partial \lambda} = \mathbf{A^T w} - \mathbf{W} = \mathbf{0} \quad (34)$$

comparing (32) and the constitutive equations (30), it follows that $\lambda = \mathbf{F}$. Using $\lambda = \mathbf{F}$ in (32) and (33), the result follows.

In principle, an optimization problem is solved where one set of Kirchhoff equations is omitted. Through the first order conditions, the missing set of equations is derived. 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.

We can now propose the main theorem which allows us to connect the steady state of a process network to the objective function that is simultaneously optimized i.e. we can find the natural optimization problem that a process network solves, when converging to a steady state. We explored the structure of the problem in the previous theorem, however, we need to be able to define boundary conditions and a solution for process networks connected to an exo-system.

Theorem 7. Consider a process network G with given resistive constitutive equations $\mathbf{F_R} = \Lambda(\mathbf{W_R})$ and boundary conditions for each terminal as well as one set of either the conservation laws or the uniqueness conditions. The stationary solution ($\frac{dZ_i}{dt} = 0$) for the network with conservation laws (13) and the uniqueness conditions (14)

$$\mathbf{AF} = \mathbf{0} \quad (35)$$

$$\mathbf{W} = \mathbf{A^T w} \quad (36)$$

$$\mathbf{F} - \mathbf{F_T} = \Lambda(\mathbf{W} - \mathbf{W_T}) \quad (37)$$

can be found by solving the following optimization problem

$$\min_{\mathbf{w}} \quad G^* = \int_0^W \mathbf{F}^T d\mathbf{W} \quad (38)$$

$$s.t. \quad \mathbf{W} = \mathbf{A^T w} \quad (39)$$

$$\mathbf{F_R} = \Lambda(\mathbf{W_R}) \quad (40)$$

$$\mathbf{F_T} = \text{const and/or } \mathbf{W_T} = \text{const} \quad (41)$$

or its equivalent dual optimization problem where (36) is replaced by (35).

Proof. Starting with (38) - (41), we substitute the boundary conditions (41) into the constitutive equations (40) and the constitutive equation into the objective function (38). We then form the Lagrange function using the flows $\mathbf{F}$ as Lagrange multipliers

$$L(\mathbf{W}, \mathbf{w}, \mathbf{F}) = \int_0^W (\Lambda(\mathbf{W} - \mathbf{W_T})^T d\mathbf{W} + \mathbf{W}^T \mathbf{F_T} \quad (42)$$

$$+ \mathbf{F}^T(\mathbf{A^T w} - \mathbf{W}) \quad (43)$$

First order conditions:

$$\frac{\partial L}{\partial \mathbf{W}} = \Lambda(\mathbf{W} - \mathbf{W_T}) + \mathbf{F_T} - \mathbf{F} = \mathbf{0} \quad (44)$$

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{AF} = \mathbf{0} \quad (45)$$

$$\frac{\partial L}{\partial \mathbf{F}} = \mathbf{A^T w} - \mathbf{W} = \mathbf{0} \quad (46)$$

Comparing (25) - (27) to (44) - (46) shows the result. Concerning the second order conditions, we observe that convexity of the constraints is trivial for the linear Kirchhoff laws. Non-convexities of the optimization problem are due to non-linearities of the constitutive equations i.e. the constitutive equations are non-positive. For the second order conditions, it is apparent that the first derivative of the constitutive equations has to be analyzed and found positive definite for a global minimum, which corresponds exactly to the findings for passivity in Jillson and Ydstie (2007) for a unique network solution and convergence.

Generally, the objective function is a measure for dissipation of the storage variable over time. We conclude that the steady state of a passive network minimizes the dissipated power subject to the constraints imposed by the constitutive equations, topology, and boundary conditions, i.e. terminal connections.

6. PIPEFLOW NETWORK

A pipeline network example shows how optimization and dynamic simulation are connected. The network consists of two connected pipelines where each pipeline flows through a cylindrical storage tank with volume V_j open to the atmosphere, as shown in Fig. 2. A reference node is introduced representing the environment and connected to the terminals and dynamic nodes.

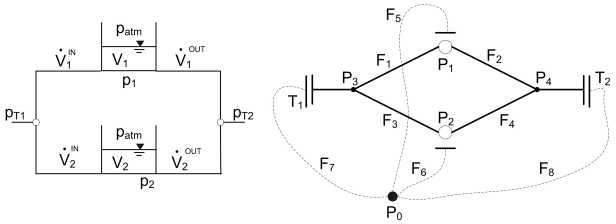

Fig. 2. Graphical network representations: Problem specific representation on the left, a generalized representation on the right including P_0 representing the exo-system.

Each pipeline's cross section is cylindrical with area A_i. The pipeline flow is given as a lumped parameter representation introducing pressure potentials p_j at the nodes and assuming laminar flow ($Re < 2300$). It is assumed that the fluid shows Newtonian behavior as well as being incompressible ($\rho = \text{const.}$). Therefore, the relation between

volumetric flow $\dot{V}_i$ and pressure drop $\Delta p_i = p_j - p_{j+1}$ can be modeled using Hagen-Poiseuille's law $\dot{V}_i = \frac{\pi r_i^4}{8\eta L_i}\Delta p_i$, where r_i is the radius of the pipeline's cross-section and L_i is the length of pipeline i. The potential at the bottom of the tank is given as $p_j = \rho g h_j + p_{atm}$ 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. We complete the model with the conservation laws for mass or, for constant density, the conservation of volume:

$$dV_1/dt = \dot{V}_1^{IN} - \dot{V}_1^{OUT} \tag{47}$$
$$dV_2/dt = \dot{V}_2^{IN} - \dot{V}_2^{OUT} \tag{48}$$
$$\dot{V}_{T1} = \dot{V}_2^{IN} + \dot{V}_2^{IN} \tag{49}$$
$$\dot{V}_{T2} = \dot{V}_2^{OUT} + \dot{V}_2^{OUT} \tag{50}$$

Initial conditions for the tank volumes $V_{0,i}$ have to be specified as well as boundary conditions at the terminals. The steady state of (47) - (50) can be found by integrating the differential equations.

The dynamic system given by the previous equations converges to the solution of the following optimization problem ($\frac{dV_1}{dt} = \frac{dV_2}{dt} = 0$):

$$\min \quad \sum_{i=1}^{4} \int_0^{\Delta p_i} \dot{V}_i d(\Delta p_i) \tag{51}$$
$$s.t. \quad (47) - (50) \tag{52}$$
$$\dot{V}_i = \frac{\pi r_i^4}{8\eta L_i}\Delta p_i \ , i = 1, .., 4 \tag{53}$$
$$\dot{V}_{T1} = const., p_{T2} = const. \tag{54}$$

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 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 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.

7. CONCLUSIONS AND DISCUSSION

We introduced a new framework for analysis of optimality and stability of networked process systems in this work. We provide a systematic approach to define stability and optimality conditions for these systems. The objective function minimized by a process systems in its steady state is derived. Although for simplicity, we regard only the steady state in this example, the optimization problem

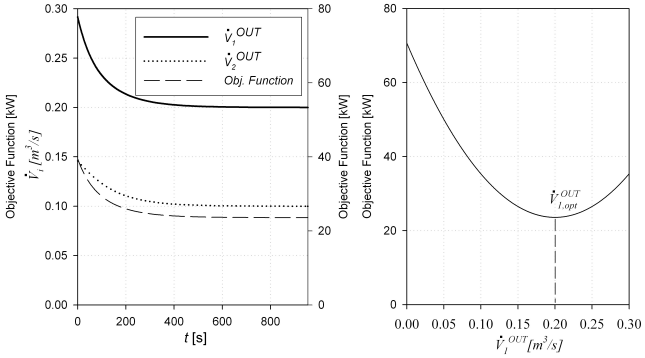

Fig. 3. Flows between tanks and outgoing terminal T_2 and the power dissipation (objective function) as a function of time on the left. Convergence of $\dot{V}_1^{OUT} =$ to 0.2 m^3/s and $\dot{V}_2^{OUT} =$ to 0.1 m^3/s. Objective function values of $\dot{V}_1^{OUT}$ on the right.

is also valid for transient conditions. The findings can explored to design decentralized control structures and hence shape the natural objective function of a process systems towards an economic objective.

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