

COMPLEX PROCESS NETWORKS: PASSIVITY AND OPTIMALITY

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Abstract: We introduce a novel modelling framework for studying dynamics, distributed control, and optimization of complex networks made up of chemical processes. We are interested in developing self-organizing structures so that stability and optimality follows as a consequence of how the networks are put together and how they are connected with boundary conditions or other networks. By considering only the topology of the system and basic conservation principles, a result analogous to Tellegen's Theorem of electrical circuit theory is produced. Using this result and passivity theory, a network is shown to converge to a stationary point when the flow relationships are positive. Also, under similar conditions, it is shown that the network is self-optimizing in that the entropy production is minimized. *Copyright*©2005 *IFAC*

1. INTRODUCTION

By developing conditions under which a process network is passive, we can show that either a system is inherently stable or how to design an effective control scheme to ensure stability. Passivity is also closely related to variational principles and can be used to demonstrate optimality. Stability and optimality are important properties to consider in a large scale integrated system like a chemical plant.

Passivity theory traces its origins to electrical circuit theory; specifically the notions that circuits with dissipative components were stable. Alonso and Ydstie (Alonso & Ydstie, 1997) outlined the conditions in which process systems have dissipative properties.

This theory could be applied to various types of networked systems previously examined with other methods, such as plant-wide (integrated) process networks (Luyben *et al.*, 1999), (Hangos *et al.*, 1999), (Gilles, 1998), (Kumar & Daou-

Fig. 1. A simple process network with four terminals, ten flows (fourteen in the complete network), and six processes, (nine in the complete network)

tidis, 2002), chemical reaction networks (Fishtik *et al.*, 2004), or biological networks (Majewski & Domach, 1989), (Hatzimanikatis *et al.*, 1996).

An important property of passivity is that interconnections of passive subsystems result in a passive overall system. Therefore, decentralization of a much larger network into smaller, more manageable subnetworks becomes feasible. Also, this allows for the addition or subtraction of various parts of the network without necessarily having to perform a stability analysis over the whole network.

2. PROCESS NETWORKS

Consider a network as shown in Figure 1, represented by a graph, $G = (F, P, T)$. F , the set

of edges, represents flow of material and energy amongst vertices and terminals. P , the set of vertices represents elementary processes. T represents the set of terminals where the network is integrated with the environment.

A network is said to be a *process network* if the following assumption holds true:

Assumption 1.

- (i) The state of an elementary process j is defined by the vector v_j .
- (ii) There exists a function, $S(v_j)$, called the entropy, which is concave.
- (iii) $S(v_j)$ is homogeneous of degree one (i.e. $\lambda S(v_j) = S(\lambda v_j)$).
- (iv) There exists at least one inventory, v_i contained in every v for which $\frac{\partial S}{\partial v_i} > 0$.

The problem we consider is

- (1) to establish conditions under which the process network is passive and
- (2) to establish a variational principle for process networks

At each node, we define intensive potentials, w , based on the entropy and extensive variables.

$$w = \frac{\partial S}{\partial v} \quad (1)$$

From this expression and Assumption 1 (iii), we develop another relationship:

Lemma 1. For an elementary process with entropy, S , extensive variables, v , and intensive variables, w ,

$$w^T v = S \quad (2)$$

$$v^T dw = 0 \quad (3)$$

Proof. Start by expanding the following partial derivative using the chain rule:

$$\frac{\partial S(\lambda v)}{\partial \lambda} = \frac{\partial S(\lambda v)}{\partial(\lambda v)} \frac{\partial \lambda v}{\partial \lambda} \quad (4)$$

From the homogeneity condition (Assumption 1, (iii)), and the fact that neither S nor v are functions of λ , Equation (4) is simplified to

$$S(v) = \frac{\lambda \partial S(v)}{\lambda \partial v} v$$

The λ 's cancel out, and using Equation (1), Equation (2) follows. By taking the partial derivative of both sides of Equation (2) with respect to v gives:

$$\frac{\partial(w^T v)}{\partial v} = \frac{\partial S}{\partial v} = w^T \quad (5)$$

Using the product rule, (5) is expanded to

$$w^T + v^T \frac{\partial w}{\partial v} = w^T \quad (6)$$

Fig. 2. Depiction of the mapping between intensive variables, w , and extensive variables, v . The w 's cancel, and Equation (3) follows, which is the generalized form of the Gibbs-Duhem equation. \square

Note that the relationships in Equation (2) provide a mapping between solutions given in intensive and extensive variables. For any elementary process in which the extensive variables are known, the exact mapping to intensive variables can be determined. However, if a set of intensive variables are known, a range of extensive variables can be determined. Therefore, for each phase in the system, one extensive variable in addition to the set of intensive variables must be known in order to fully specify. This can be seen graphically in Figure 2.

Let n_t represent the number of terminals, n_p the number of processes, n_f the number of edges, and n the number of distinct material components. At each vertex and terminal in the network, a balance of the extensive variables holds true so that:

$$\frac{dv_j}{dt} = p_j + \sum_{i=0, i \neq j}^{n_t+n_p} f_{ij}, \quad j = 1, \dots, n_t + n_p \quad (7)$$

p_j is the $n + 2$ vector of production rates (e.g. changes in mass/energy due to chemical reaction) at node j , and f_{ij} is the $n + 2$ vector of flows of energy, volume, and mass from node i to node j , and is equal to zero when no connection is defined. Thus, there are no more than n_f non-zero vector flows in the network.

If we view the connection between any two nodes as a one-dimensional segment (e.g. pipe) of length L_{ij} , then we can define a change in potential from node i to node j as:

$$W_{ij} = \int_0^{L_{ij}} \left(\frac{\partial w}{\partial x} \right) dx \quad (8)$$

in which $\frac{\partial w}{\partial x}$ denotes the local gradient. By using the fundamental theorem of calculus, Equation (8) can be simplified to

$$W_{ij} = w_i - w_j \quad (9)$$

These potential differences, W_{ij} , act as driving forces that cause flow in the network. The actual flows are given by constitutive relationships of the form

$$f = \Lambda(u)W$$

where u is a control/optimization parameter and $\Lambda(u)$ is a matrix function.

Since the variables W_{ij} are continuous, around any closed loop we have

$$\oint \left(\frac{\partial w}{\partial x} \right) dx = 0 \quad (10)$$

Fig. 3. A network showing the connections of the terminals to a reference (ground) state.

Equation (10) is analogous to Kirchoff's voltage law for electrical networks for a multi-component system, while Equation (7) is analogous to Kirchoff's current law.

3. A TOPOLOGICAL RESULT

In this section, we develop a property of process networks which only relies on topological properties. We also introduce the concept of network operators, which allows us to generalize the topological result to cover a wide range of network applications. For example, in the next section, we use the generalized result to establish sufficient conditions for the stability of process networks using thermodynamics and passivity theory.

Lemma 2. For two process networks, (a) and (b), with the same topology and (possibly) differing operating conditions,

$$\sum_{j=1}^{n_p} w_j^{bT} \frac{dv_j^a}{dt} = \sum_{j=1}^{n_p} w_j^{bT} p_j^a + \sum_{k=1}^{n_f} W_k^{bT} f_k^a + \sum_{j=1}^{n_t} w_j^{bT} f_j^a \quad (11)$$

Proof: Beginning with Equation (7) for each process and terminal in network a:

$$\frac{dv_j^a}{dt} = p_j^a + \sum_{i=0, i \neq j}^{n_p+n_t} f_{ij}^a \quad (12)$$

$$j = 0, \dots, n_p + n_t$$

In this equation, the flow from every other process or terminal in the system into process or terminal j is considered. For most networks, especially very large ones, most of these flows will be zero. Also, it should be noted that we have an introduced an extra node, indexed by 0. This node, which satisfies Equation (7), considers the flow into or out of the terminals from outside the network, as shown in Figure 3. This node has a fixed reference potential, assumed to be equal to zero. Next, by multiplying equation (12) by the potential, w_j of network b gives

$$w_j^{bT} \frac{dv_j^a}{dt} = w_j^{bT} p_j^a + \sum_{i=0, i \neq j}^{n_p+n_t} w_j^{bT} f_{ij}^a \quad (13)$$

$$j = 0, \dots, n_p + n_t$$

Taking the summation of Equation (13) over all processes, terminals, and the zero node gives

$$\sum_{i=0}^{n_p+n_t} w_j^{bT} \frac{dv_j^a}{dt} = \sum_{i=0}^{n_p+n_t} w_j^{bT} p_j^a + \sum_{i=0}^{n_p+n_t} \sum_{i=0, i \neq j}^{n_p+n_t} w_j^{bT} f_{ij}^a \quad (14)$$

Since no storage or production occurs at the terminals, and that the potential of the zero node is assumed to be zero, Equation (14) is simplified to

$$\sum_{j=1}^{n_p} w_j^{bT} \frac{dv_j^a}{dt} = \sum_{j=1}^{n_p} w_j^{bT} p_j^a + \sum_{j=0}^{n_p+n_t} \sum_{i=0, i \neq j}^{n_p+n_t} w_j^{bT} f_{ij}^a \quad (15)$$

Using the fact that $f_{ij} = -f_{ji}$, and that flow only occurs through connected nodes/terminals, Equation (11) follows, where f_k^a is the subset of f_{ij}^a made up of only positive internal flows. \square

For a steady state system with no terminals and no production, Equation (11) implies that the vector product of flows (f) and driving forces (W) are orthogonal.

In order to facilitate further proofs, we introduce the following definition:

Definition 1. Operators ($\Gamma_v, \Gamma_f, \Gamma_W$) are called network operators provided Equations (7) and (10) hold for the transformed variables, $\bar{v} = \Gamma_v v$, $\bar{f} = \Gamma_f f$, $\bar{p} = \Gamma_p p$, $\bar{W} = \Gamma_W W$, and $\bar{w} = \Gamma_w w$

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.

Corollary 1. Since Lemma 2 is based only on the topology of the system, with the conservation equations (7),(10), transformed variables (\bar{v} , \bar{W} , \bar{w} , and \bar{f}) can be substituted into Equation (11) and the result holds true.

4. PASSIVITY

In order to show the stability of a process network, we will exploit passivity theory (Byrnes *et al.*, 1991). A system with state x is passive if there exists a *positive semi-definite* storage function, V , that satisfies the passivity inequality:

$$V(x(t)) \leq V(x(0)) + \int_0^t u^T y ds - \epsilon_0 \int_0^t x^T x ds \quad (16)$$

with $V(x) \geq 0$ if $|x| \neq 0$ and $V(x) = 0$ if $|x| = 0$. x is the vector of states, u the vector of inputs, y the vector of outputs, and ϵ_0 is a positive constant.

In a process network there exists a natural storage function based on the entropy. At each process

node we define a scalar storage function, $g(v_1, v_2)$ based on the potentials and inventories:

$$g(v_1, v_2) = (v_1 - v_2)^T (w_2(v_2) - w_1(v_1)) \quad (17)$$

This storage function provides a way to determine how far away one solution (v_1, w_1) is from another (v_2, w_2) . One solution could for example be a stationary point or an oscillating solution. Passivity would then address if the second solution converges to the first. Defining deviation variables

$$\bar{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \quad \bar{w} = \begin{pmatrix} w_1 - w_2 \\ w_2 - w_1 \end{pmatrix}$$

Using these variables, Equation (17) can be rewritten as

$$g(\bar{v}) = -\bar{w}^T \bar{v} \quad (18)$$

Recall from definition (1, ii) that entropy is a strictly concave function of v and from equation (1) that the derivative with respect to v defines the potentials, w . It can be easily seen that for any pair v_1, v_2 :

$$g(\bar{v}) > 0 \quad |\bar{w}| \neq 0$$

and

$$g(\bar{v}) = 0 \quad |\bar{w}| = 0$$

An overall storage function of the network, $G(t)$ is defined at time t as:

$$G(t) = G(v_1(t), v_2(t)) = \sum_{i=1}^{n_p} g_i(v_1, v_2) \quad (19)$$

Lemma 3. For a network in which the entropy function, $S(v)$, is concave then:

$$\frac{dG}{dt} = - \sum_{k=1}^{n_f} \bar{W}_k^T \bar{f}_k - \sum_{j=1}^{n_p} \bar{w}_j^T \bar{p}_j - \sum_{j=1}^{n_t} \bar{w}_j^T \bar{f}_j \quad (20)$$

Proof: Starting by taking the derivative of $g(\bar{v})$ which gives:

$$\frac{dg}{dt} = - \frac{d\bar{w}^T}{dt} \bar{v} - \bar{w}^T \frac{d\bar{v}}{dt} \quad (21)$$

From Equation (3), the first term in the RHS is equal to zero. Therefore

$$\frac{dg}{dt} = -\bar{w}^T \frac{d\bar{v}}{dt} \quad (22)$$

By summing over all the nodes we get:

$$\frac{dG}{dt} = - \sum_{i=1}^{n_p} \bar{w}_i^T \frac{d\bar{v}_i}{dt} \quad (23)$$

By using Equation (11) and Corollary (1), Equation (23) can be rewritten as Equation (20). \square

If we assume

$$\sum_{k=1}^{n_f} \bar{W}_k^T \bar{f} + \sum_{j=1}^{n_p} \bar{w}_j^T \bar{p}_j \geq \epsilon_0 \sum_{j=1}^{n_p} \bar{w}_j^T \bar{w}_j \quad (24)$$

and by integrating Equation (20), we get

$$G(t) \leq G(0) - \epsilon_0 \int_0^t \sum_{j=1}^{n_p} \bar{w}_j^T \bar{w}_j - \int_0^t \sum_{j=1}^{n_t} \bar{w}_j^T \bar{f}_j \quad (25)$$

If we set

$$\bar{w}_{terminals} \mapsto y$$

$$\bar{f}_{terminals} \mapsto u$$

$$\bar{w}_{nodes} \mapsto x$$

then the network is clearly passive. Note that the mapping of control variables u and output variables y can be interchanged, depending on the desired output of the network. Inequality (24) is true if the monotonicity relationships:

$$\bar{W}^T \bar{f} \geq \epsilon_1 \bar{W}^T \bar{W} \quad \bar{p}^T \bar{w} \geq \epsilon_2 \bar{w}^T \bar{w} \quad (26)$$

are satisfied and is further relaxed by using a discrete form of the Poincaré inequality similar to one given by Straughan (Straughan, 1992). Some physical examples where the inequalities (26) hold are given for electrical circuits by Penfield et al (Penfield *et al.*, 1970) and for reaction and diffusion systems by Kreuzer (Kreuzer, 1981).

5. OPTIMALITY

Assume a network is characterized by a solution, x^* . This solution fixes the flows between nodes, f^* , potentials, w^* , (and consequently the potential differences, W^*), the production rates, p^* , and the inventories, v^* , all at each node. Using a definition of entropy production given by Ydstie (Ydstie, 2002), we have

$$\sigma_s = \int_0^f W(\hat{f}) d\hat{f} + \int_0^p w(\hat{p}) d\hat{p} \quad (27)$$

Given certain classes of constitutive relationships defining flow and production rates based on potential differences and potentials, respectively, then we develop following result.

Lemma 4. Supposing that the monotonicity relationships (26) hold, the solution of a network, x^* , obeying balance equations (7),(10) compared to a finitely perturbed network, x , minimizes entropy production, as given by the following inequality

$$\int_0^t \sum_{k=1}^{n_f} \alpha_k dt + \int_0^t \sum_{i=1}^{n_p} \beta_i dt \geq \int_0^t \sum_{k=1}^{n_f} \alpha_k^* dt + \int_0^t \sum_{i=1}^{n_p} \beta_i^* dt \quad (28)$$

with

$$\alpha_k = \int_0^{f_k} W_k(f) df \quad \beta_i = \int_0^{p_i} w_i(p) dp$$

Proof: We start by allowing the flows (within the network), and production rates to differ from those given by x^* (at some time, $t = 0$), while

keeping the potentials and inventories (w^*, v^* respectively) fixed. These deviations in extensive variables must still obey Equation (7). Equation (11) for one network is

$$\sum_{j=1}^{n_p} w_j^T \frac{dv_j}{dt} = \sum_{j=1}^{n_p} w_j^T p_j + \sum_{k=1}^{n_f} W_k^T f_k + \sum_{j=1}^{n_t} w_j^T f_j \quad (29)$$

We define the time derivative of entropy S , using the chain rule and Equation (1) to give:

$$\frac{dS}{dt} = \frac{dS}{dv} \frac{dv}{dt} = w^T \frac{dv}{dt} \quad (30)$$

Substituting this into (29) gives

$$\sum_{j=1}^{n_p} \frac{dS_j}{dt} = \sum_{j=1}^{n_p} w_j^T p_j + \sum_{k=1}^{n_f} W_k^T f_k + \sum_{j=1}^{n_t} w_j^T f_j \quad (31)$$

Recalling from Corollary (1), that deviation variables can substituted into Equation (11), we define the following deviation variables:

$$\begin{aligned} \bar{w} &= w^* & \bar{W} &= W^* & \bar{f} &= f - f^* \\ \bar{p} &= p - p^* & \bar{S} &= S - S^* \end{aligned}$$

Substituting these into (31) and integrating gives

$$\begin{aligned} \sum_{i=1}^{n_p} \bar{S}(t) &= \int_0^t \sum_{j=1}^{n_p} \bar{w}_j^T \bar{p}_j dt + \int_0^t \sum_{k=1}^{n_f} \bar{W}_k^T \bar{f}_k dt \\ &\quad + \int_0^t \sum_{j=1}^{n_t} \bar{w}_j^T \bar{f}_j dt \end{aligned} \quad (32)$$

Since the flows at the terminals are fixed, the last term goes to zero, since $\bar{f}_j = f_j - f_j^* = 0$ at all the terminals. From monotonicity relationships (26), we have:

$$\int_f^{f^*} (W^* - W(f)) df \geq 0 \quad (33)$$

$$\int_p^{p^*} (w^* - w(p)) dp \geq 0 \quad (34)$$

where $W(f)$ and $w(p)$ define potential differences and potentials for which the flow/production is equal to f or p as given by the constitutive relationship (e.g. $W(f^*) = W^*$).

Since W^* is constant, Equation (33) is rewritten as

$$W^{*T}(f^* - f) \geq \int_f^{f^*} W(f) df$$

and subsequently

$$W^{*T}(f^* - f) \geq \int_0^{f^*} W(f) df - \int_0^f W(f) df$$

Recalling the definition of α and deviation variables \bar{W} and \bar{f} this is simplified to

$$\bar{W}^T \bar{f} \geq \alpha^* - \alpha \quad (35)$$

A similar transformation is performed on (34) to give

$$\bar{w}^T \bar{p} \geq \beta^* - \beta \quad (36)$$

Substituting (35) and (36) into (32) gives

$$\begin{aligned} \sum_{i=1}^{n_p} \bar{S}(t)_i &\geq \int_0^t \sum_{k=1}^{n_f} (\alpha_k^* - \alpha_k) dt + \\ &\quad \int_0^t \sum_{i=1}^{n_p} (\beta_i^* - \beta_i) dt \end{aligned} \quad (37)$$

Writing this in deviation form gives:

$$\begin{aligned} \sum_{i=1}^{n_p} S_i(t) &+ \int_0^t \sum_{k=1}^{n_f} \alpha_k dt + \int_0^t \sum_{i=1}^{n_p} \beta_k dt \geq \\ \sum_{i=1}^{n_p} S_i(t)^* &+ \int_0^t \sum_{k=1}^{n_f} \alpha_k^* dt + \int_0^t \sum_{i=1}^{n_p} \beta_k^* dt \end{aligned} \quad (38)$$

Also, since the potentials and the inventories of both the simulated and deviated networks are the same at all times, we have $S_i^* = S_i$ for all $i = [1, n_p]$. Using this, we derive Equation (28). \square

Using the expression for entropy production, Equation (27), this can be interpreted to show that the entropy production of the whole network over time $t = [0, t]$ will never be less in a deviated network compared to the network governed by solution, x^* . Also, we could easily show a similar result by fixing the flows and varying the potentials within the network.

6. CONCLUSIONS

A modelling framework has been developed to describe complex networks of chemical processes. The framework is based largely on fundamental ideas from thermodynamics, including the use of an entropy function, as well as flows or production of extensive variables based on potentials or potential differences. Using a storage function based on entropy is used to develop passivity of the network. By establishing passivity, a network can easily be stabilized using feedback control. Also, for finite perturbations in flows and production rates, it was shown that the network that obeys the constitutive laws will never have a higher entropy production than the deviated network. These two properties (passivity and optimality) were demonstrated in two examples. Another example was used to illustrate a sufficient condition for both

the optimality and passivity results. Some possible applications include plant-wide control, real time process optimization, bio-chemical metabolic networks, and supply chain management.

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7. NOMENCLATURE

n_p - the number of processes in the network
 n_t - the number of terminals in the network
 n_f - the number of flows between processes and/or terminals
 f_{ij} - the vector containing flows from node or terminal i to node or terminal j
 f_j - the vector containing flows into (positive) or out of (negative) terminal j
 w_j - the vector of potentials at node or terminal j
 W_k - vector of potential differences for connection k
 p_j - production vector at node or terminal j
 v_j - inventory vector at node or terminal j
 S_j - Entropy at node or terminal j
 $\sigma_{s,j}$ - Entropy production at node or connection j
 Λ - Diffusivity coefficient matrix

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