Process Networks with Chemical Engineering Applications

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Objectives

- Describe a systematic framework for modeling process networks
- Develop passivity based methods for stability analysis and control of process networks
- Establish a variational principle for process networks
- Develop a reactor-diffusion network and a plant-wide control case study
Process Networks

Define

- Graph, $G = (P, T, F)$
  - Process (node)
  - Terminal
  - Flow
- Inventory of each node, $v_j$
  - Extensive quantities, conserved at each node
  - e.g. $v = [U, V, M_1, ..., M_n, ...]^T$
- Potential of each node, $w_j$
  - Intensive quantities, continuous around any loop
  - e.g. $w = \left[ \frac{1}{T}, \frac{P}{T}, \frac{\mu_1}{T}, ..., \frac{\mu_n}{T}, ... \right]^T = \frac{\partial S}{\partial v}$
  - Potential differences ($W$) act as driving forces for flow through constitutive relationships
Examples of Process Networks

- Supply Chain Networks
- Process Flowsheets
- Biological Systems
- Chemical Reaction Pathways
Passivity Background

- Passivity theory is used to show network stability
  - Originated from electrical circuit theory
  - A feedback or parallel connected system of passive subsystems is also passive
- Passivity inequality
  \[
  \frac{dV(x)}{dt} \leq u^T y - \epsilon_0 x^T x
  \]
  - With \( x, u, y \) the states, inputs, and outputs to the network
  - \( V(x) \geq 0, x \neq 0; V(0) = 0 \)
  - Network is strictly passive if \( \epsilon_0 > 0 \)
- Problem: To find a practical storage function
Exploitation of Entropy to Develop a Storage Function

Tangent line with slope $w^*$

- $a(v_1) > 0$, $w \neq w^*$
- $a(v) = 0$, $w = w^*$
Storage Function Defined

- At each node:
  \[ a(v) = w^T(v - v^*) - (S(v) - S(v^*)) \geq 0 \]

- For the whole network
  \[ A(t) = \sum_{i=1}^{n_p} a_i(v_i) \geq 0 \]

- Differentiation and using deviation variables gives
  \[ \frac{dA}{dt} = \sum_{j=1}^{n_p} -\bar{w}_j \frac{d\bar{v}_j}{dt} \]
Use a result similar to Tellegen’s Theorem (Proof shown in Jillson, Ydstie 2005)

\[ \sum_{j=1}^{n_p} w_j^T \frac{dv_j}{dt} = \sum_{j=1}^{n_p} w_j^T p_j + \sum_{k=1}^{n_f} W_k^T f_k + \sum_{j=1}^{n_t} w_j^T f_j \]

- Based only on topology of network

Substituting into the previous equation

\[ \frac{dA}{dt} = - \sum_{k=1}^{n_f} W_k^T \bar{f}_k - \sum_{j=1}^{n_p} \bar{w}_j^T \bar{p}_j - \sum_{j=1}^{n_t} \bar{w}_j^T \bar{f}_j \]

- Flow between nodes
- Production within nodes
- Boundary conditions
Passivity of Process Networks

- If

\[
\sum_{k=1}^{n_f} \overline{W}_k^T \bar{f} + \sum_{j=1}^{n_p} \overline{w}_j^T \bar{p}_j \geq \epsilon_0 \sum_{j=1}^{n_p} \overline{w}_j^T \overline{w}_j
\]

Then

\[
\frac{dA}{dt} \leq - \sum_{j=1}^{n_t} \overline{w}_j^T \bar{f}_j - \epsilon_0 \sum_{j=1}^{n_p} \overline{w}_j^T \overline{w}_j \quad \rightarrow \quad \text{Network is Strictly Passive!}
\]

\[
\begin{align*}
\text{True for positive constitutive flow and production rates}
\end{align*}
\]
Multi-component Flow

$w_1 \xrightarrow{f_{12}} w_2$

- Inventories and Potentials

$$v = [U, V, M_1, \ldots, M_n] \quad w = \left[ \frac{1}{T}, \frac{P}{T}, -\frac{\mu_1}{T}, \ldots, -\frac{\mu_n}{T} \right]$$

- Convective and Diffusive Flow

$$f = -k \hat{z} \frac{\partial P}{\partial x} - \Lambda \frac{\partial w}{\partial x} \quad k > 0 \quad \Lambda > 0$$

$$\hat{z} = [\hat{H}, z_1, \ldots, z_n]$$

$$\hat{H} = \hat{U} + PV$$
Using the Gibbs-Duhem equation

\[ 0 = \frac{\hat{V}}{T} dP + \hat{H} d\left(\frac{1}{T}\right) + \hat{z} d\left(-\frac{\mu}{T}\right) \quad \Rightarrow \quad -\frac{dP}{dx} = \frac{T}{\hat{V}} (\hat{z} d\left(-\frac{\mu}{T}\right) + \hat{H} d\left(\frac{1}{T}\right)) \]

- Plugging in this expression into the flow equation and integrating over a length, \( L \), gives:

\[ f = \left( < \frac{k}{\hat{V}} T \hat{z} \hat{z}^T > + < \Lambda > \right) W = \Delta W \]

- Potential Flow relationship is positive
Reactor-Distillation Model
(similar to Kumar and Daoutidis, 2002)

- Reactor Model: CSTR:
  A → B → C with 1\textsuperscript{st} order kinetics

- Distillation Model:
  - CMO
  - 15 trays
  - Saturated Liquid Feed on 4\textsuperscript{th} tray
  - Constant Relative volatilities \{4,2,1\}

- Fixed Feed rate and purge ratio

- 10 flows, 5 units (not counting flows within the distillation column)
Pressure driven flows

- Mass of each species in each unit \( \rightarrow \) inventory
- Introduce the pressure of each unit as a function of the total mass \( \rightarrow \) potential
  - Bulk flow between units would be a linear function of the differences in pressure \( f_{ij} = k_{ij}(P_i - P_j) \)
  - Control laws could be written to derive the \( k \) values, e.g:
    \[
    k_f = \frac{F_0 + R_c + K_f(N_r - N_r^{sp})}{P_r - P_{dc}}
    \]
  - Problems arise with recycle loops, due to non passive pump units
Inventory Controllers

- For total mass in four units

\[
F = F_0 + R_c + K_f(N_r - N_r^{sp}) \\
B = L - V + K_b(N_b - N_b^{sp}) \\
D = V - R + K_d(N_d - N_d^{sp}) \\
R_c + P = D + K_p(N_p - N_p^{sp})
\]

- At steady state, these become units’ mass balances
- Account for 4 degrees of freedom, leaving 6 remaining
Remaining Degrees of Freedom

- Inventory control on single component (A) in reboiler
  \[ V = \frac{1}{y_b^A}(Lx_{15}^A - Bx_b^A + K_v(N_b^A - N_b^{Asp})) \]

- Fixed Feed rate
- Fixed Purge Ratio
- Fixed Reflux
- Mass Balance Constraints on Distillation Column
  \[ V_{bottom} = V_{top} \]
  \[ L = F + R \]
Simulation Results

- For a step change in the fixed feed rate (at \( t=500 \) from \( F_0 = 100 \) to 150) and a change in the set point of the number of moles of A in the reboiler (at \( t = 1000 \) from \( N_{b}^{A, sp} = 9 \) to 2 (in effect changing \( x^A \) from 0.050 to 0.011):
Variational Principle for Process Networks

- Define the entropy production

\[ \sigma_s(f) = \int_0^{f_k} W(\hat{f})d\hat{f} \quad \text{→ Contribution due to flow} \]

\[ \sigma_s(p) = \int_0^{p_k} w(\hat{p})d\hat{p} \quad \text{→ Contribution due to production} \]

- For the complete network

\[ \sigma_s(f, p) = \sum_{k=1}^{n_f} \sigma_s(f_k) + \sum_{i=1}^{n_p} \sigma_s(p_i) \geq 0 \]
Optimality

Theorem: The total entropy production is minimized along all system trajectories

\[
\int_0^t \sum_{k=1}^{n_f} \sigma_s(f_k) + \sum_{i=1}^{n_p} \sigma_s(p_i) dt \geq \int_0^t \sum_{k=1}^{n_f} \sigma_s(f_k^*) + \sum_{i=1}^{n_p} \sigma_s(p_i^*) dt
\]

for fixed node and terminal potentials, and positive monotonic constitutive expressions

(Proof in Jillson, Ydstie 2005)
Reactor Network Example

- Three reactor nodes, and three terminals
  - Reaction: A + B \rightarrow C
  - Transport governed by diffusion

\[
\frac{dv_i}{dt} = \sum f_{ij} + p_i
\]

9 ODE’s

27 Algebraic constitutive

\[
f_{ij} = L_{ij}(C_i - C_j)
\]

\[
p_{ik} = \nu_k k^T C_i
\]
Control of Example

- **Objective**: Control flow rate of C at T3
- **Stabilized by a PI flow controller** ($K = 50$, $1/\tau = 10$) to a set point, $f_{c}(3) = 0.05$
  \[ f_{C}(3) \rightarrow y \quad \text{L3,3 of } f_{C} \rightarrow u \]
Optimality Result

- Minimal entropy production in unperturbed solution, compared to a randomly perturbed network
Conclusions

- Process Networks modeled as a graph with state $v$ and potential $w$ at each node.
- Storage function, $A$, used to show passivity provided flow and production rates are monotonic and positive.
- Simulation examples presented to demonstrate theory.
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